201-15585B

APPENDIX II

ROBUST SUMMARIES OF STUDIES USED TO CHARACTERIZE THE LOW 1,3-BUTADIENE C4 CATEGORY

PHYSICO-CHEMICAL ROBUST SUMMARIES

Melting Point

Test Substance:	Other TS [CAS # 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5]
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Melting Point is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of K. Joback and Gold and Ogle. Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. The Gold and Ogle Method simply uses the formula Tm = 0.5839Tb, where Tm is the melting point in Kelvin and Tb is the boiling point in Kelvin.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured melting point data for representative constituents of the Low 1,3-Butadiene C4 Category are listed below. The data identify a potential melting point range for substances represented by the eight CAS numbers under Test Substance. Substances in this category do not have a specific melting point value. Actual melting point of substances in this category will vary dependent on their constituent composition.

	Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C4. The eight chemicals selected to represent the melting point range of this category are C4 hydrocarbons that can be found in substances identified by the eight CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, olefinic process (distillation) knowledge, and percentage of the composition of the represented process streams. Substance Constituent / Calculated MP (°C) / Measured* MP (°C) Isobutane -132.55 -138.3 n-Butane -120.28 -138.2 Isobutylene -130.88 -140.4 cis-Butene-2 -120.41 -105.5 trans-Butene-2 -120.41 -105.5 Butene-1 -121.74 -145.0 1,2-Butadiene -117.86 -136.2 1,3-Butadiene -123.21 -108.9 * Experimental values from EPIWIN database. The data represent a potential melting point range for substances represented by the eight CAS numbers under Test Substance.
Test Substance:	The Low 1,3-Butadiene C4 Category includes the following CAS numbers: 106-97-8 Butane 106-98-9 1-Butene 115-11-7 1-Propene,2-methyl 25167-67-3 Butenes 68477-42-9 Gases, petroleum, extractive, C3-5, butene-isobutylene-rich 68477-83-8 Gases, petroleum, C3-5 olefinic-paraffinic alkylation feed 68527-19-5 Hydrocarbons, C1-4, debutanizer fraction 68606-31-5 Hydrocarbons C3-5, butadiene purification by-product

	Low 1,3-Butadiene C4 Category substances arise from production processes associated with ethylene manufacturing. The eight CAS numbers are used to describe the seven process streams arising from the ethylene process, associated butadiene purification process and other related C4 processes. Four of these process streams are complex mixtures while the remaining three describe high purity hydrocarbons. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent. With the exception of CAS 106-97-8 (butane) these substances contain significant levels of olefins. More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	Based on calculated constituent data, substances in this category can have a melting range of -117.86 to -120.28 °C. Based on measured constituent data, substances in this category can have a melting range of -145.0 to -105.5°C.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential melting point range for substances represented by the eight CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low 1,3-Butadiene C4 Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for melting point range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Melting point values were calculated by the MPBPWIN subroutine and measured data came from the database in the computer program.)

Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

Boiling Point

Test Substance:	Other TS [CAS # 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5]
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Pressure:	760 mm Hg
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Boiling Point is calculated by the MPBPWIN subroutine, which is based on the method of S. Stein and R. Brown in "Estimation of Normal Boiling Points from Group Contributions". 1994. J. Chem. Inf. Comput. Sci. 34: 581-587.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured boiling point data for representative constituents of the Low 1,3-Butadiene C4 Category are listed below. The data identify a potential boiling point range for substances represented by the eight CAS numbers under Test Substance. Substances in this category do not have a specific boiling point value. Actual boiling point ranges for substances in this category will vary dependent on their constituent composition. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C4. The eight chemicals selected to represent the boiling point range of this category are C4 hydrocarbons that can be found in substances identified by the eight CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, olefinic process (distillation) knowledge, and percentage of the composition of the represented process streams.

	Substance Constituent / Calculated BP (°C) / Measured* BP (°C) Isobutane 3.21 -11.7 n-Butane 19.58 -0.5 Isobutylene 10.18 -6.9 cis-Butene-2 27.82 0.8 trans-Butene-2 27.82 0.8 Butene-1 17.57 -1.3 1,2-Butadiene 19.71 10.9 1,3-Butadiene 15.55 -4.4 * Experimental values from EPIWIN database. The data represent a potential boiling point range for substances represented by the eight CAS numbers under Test Substance.
Test Substance:	The Low 1,3-Butadiene C4 Category includes the following CAS numbers: 106-97-8 Butane 106-98-9 1-Butene 115-11-7 1-Propene,2-methyl 25167-67-3 Butenes 68477-42-9 Gases, petroleum, extractive, C3-5, butene-isobutylene-rich 68477-83-8 Gases, petroleum, C3-5 olefinic-paraffinic alkylation feed 68527-19-5 Hydrocarbons, C1-4, debutanizer fraction 68606-31-5 Hydrocarbons C3-5, butadiene purification by-product Low 1,3-Butadiene C4 Category substances arise from production processes associated with ethylene manufacturing. The eight CAS numbers are used to describe the seven process streams arising from the ethylene process, associated butadiene purification process and other related C4 processes. Four of these process streams are complex mixtures while the remaining three describe high purity hydrocarbons. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent. With the exception of CAS 106-97-8 (butane) these substances contain significant levels of olefins.

	More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	Based on calculated constituent data, substances in this category can have a boiling range of 3.21 to 27.82°C @ 760 mm Hg. Based on measured constituent data, substances in this category can have a boiling range of -11.7 to 10.9°C @ 760 mm Hg.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential boiling point range for substances represented by the 8 CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low 1,3-Butadiene C4 Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for boiling point range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Boiling point values were calculated by the MPBPWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

Vapor Pressure

Test Substance:	Other TS [CAS # 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5]
Method/Guideline:	Calculated values using MPBPWIN version 1.40, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Vapor Pressure is calculated by the MPBPWIN subroutine, which is based on the average result of the methods of Antoine and Grain. Both methods use boiling point for the calculation. The Antoine Method is described in the Handbook of Chemical Property Estimation. Chapter 14. W.J. Lyman, W.F. Reehl and D.H. Rosenblatt, Eds. Washington, D.C.: American Chemical Society. 1990. A modified Grain Method is described on page 31 of Neely and Blau's Environmental Exposure from Chemicals, Volume 1, CRC Press. 1985.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured vapor pressure data for representative constituents of the Low 1,3-Butadiene C4 Category are listed below. The data identify a potential vapor pressure for substances represented by the eight CAS numbers under Test Substance. Substances in this category do not have a specific vapor pressure value. Actual vapor pressure of substances in this category will vary dependent on their constituent composition. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C4. The eight chemicals selected to represent the vapor pressure range of this category are C4

	hydrocarbons that can be found in substances identified by the eight CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, olefinic process (distillation) knowledge, and percentage of the composition of the represented process streams. Substance Constituent / Calculated VP (hPa @ 25°C) / Measured* VP (hPa @ 25°C) Isobutane: 3.45 E^3 / 3.08 E^3 n-Butane: 2.41 E^3 / 2.43 E^3 Isobutylene: 2.97 E^3 / 3.08 E^3 cis-Butene-2: 2.31 E^3 / 2.33 E^3 trans-Butene-2: 2.31 E^3 / 2.33 E^3 Butene-1: 2.48 E^3 / 3.00 E^3 1,2-Butadiene: 1.65 E^3 / 1.68 E^3 1,3-Butadiene: 2.73 E^3 / 2.81 E^3 * Experimental values from EPIWIN database. The data represent a potential vapor pressure range for substances represented by the eight CAS numbers under Test Substance.
Test Substance:	The Low 1,3-Butadiene C4 Category includes the following CAS numbers: 106-97-8 Butane 106-98-9 1-Butene 115-11-7 1-Propene,2-methyl 25167-67-3 Butenes 68477-42-9 Gases, petroleum, extractive, C3-5, butene-isobutylene-rich 68477-83-8 Gases, petroleum, C3-5 olefinic-paraffinic alkylation feed 68527-19-5 Hydrocarbons, C1-4, debutanizer fraction 68606-31-5 Hydrocarbons C3-5, butadiene purification by-product Low 1,3-Butadiene C4 Category substances arise from production processes associated with ethylene manufacturing. The eight CAS numbers are used to describe the seven process streams arising from the ethylene process, associated butadiene purification process and other related

	C4 processes. Four of these process streams are complex mixtures while the remaining three describe high purity hydrocarbons. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent. With the exception of CAS 106-97-8 (butane) these substances contain significant levels of olefins. More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	Based on calculated constituent data, substances in this category can have a vapor pressure range of 1.65 E^3 to 3.45 E^3 hPa @ 25°C. Based on measured constituent data, substances in this category can have a vapor pressure range of 1.68 E^3 to 3.08 E^3 hPa @ 25°C.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential vapor pressure range for substances represented by the eight CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low 1,3-Butadiene C4 Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for vapor pressure range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Vapor pressure values were calculated by the MPBPWIN subroutine and measured data came from the database in the computer program.)

Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

Partition Coefficient

Test Substance:	Other TS [CAS # 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5]
Method/Guideline:	Calculated values using KOWWIN version 1.65, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Octanol / Water Partition Coefficient is calculated by the KOWWIN subroutine, which is based on an atom/fragment contribution method of W. Meylan and P. Howard in "Atom/fragment contribution method for estimating octanol-water partition coefficients". 1995. *J. Pharm. Sci*. 84:83-92.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured log K_{ow} data for representative constituents of the Low 1,3-Butadiene C4 Category are listed below. The data identify a potential log K_{ow} range for substances represented by the eight CAS numbers under Test Substance. Substances in this category do not have a specific log K_{ow} value. Actual log K_{ow} ranges for substances in this category will vary dependent on their constituent composition. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C4. The eight chemicals selected to represent the log K_{ow} range of this category are C4 hydrocarbons that can be found in substances identified by the eight CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, olefinic process (distillation) knowledge, and percentage of the composition of the represented process streams.

	Substance Constituent / Calculated log K_{ow} @ 25°C / Measured* log K_{ow} @ 25°C Isobutane 2.23 2.76 n-butane 2.31 2.89 isobutylene 2.23 2.34 cis-butene-2 2.09 2.31 trans-butene-2 2.09 2.33 butene-1 2.17 2.40 1,2-butadiene 2.06 na 1,3-butadiene 2.03 1.99 * Experimental values from EPIWIN database. na = not available The data represent a potential log K_{ow} range for substances represented by the eight CAS numbers under Test Substance.
Test Substance:	The Low 1,3-Butadiene C4 Category includes the following CAS numbers: 106-97-8 Butane 106-98-9 1-Butene 115-11-7 1-Propene,2-methyl 25167-67-3 Butenes 68477-42-9 Gases, petroleum, extractive, C3-5, butene-isobutylene-rich 68477-83-8 Gases, petroleum, C3-5 olefinic-paraffinic alkylation feed 68527-19-5 Hydrocarbons, C1-4, debutanizer fraction 68606-31-5 Hydrocarbons C3-5, butadiene purification by-product Low 1,3-Butadiene C4 Category substances arise from production processes associated with ethylene manufacturing. The eight CAS numbers are used to describe the seven process streams arising from the ethylene process, associated butadiene purification process and other related C4 processes. Four of these process streams are complex mixtures while the remaining three describe high purity hydrocarbons. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent. With the exception of CAS 106-97-8 (butane) these substances contain significant levels of olefins.

	More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	Based on calculated constituent data, substances in this category can have a log K_{ow} range of 2.03 to 2.31 @ 25°C. Based on measured constituent data, substances in this category can have a log K_{ow} range of 1.99 to 2.89 @ 25°C.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential log K_{ow} range for substances with the eight CAS numbers listed under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low 1,3-Butadiene C4 Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for log K_{ow} range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Log K_{ow} values were calculated by the KOWWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

Water Solubility

Test Substance:	Other TS [CAS # 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5]
Method/Guideline:	Calculated values using WSKOWWIN version 1.36, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Water Solubility is calculated by the WSKOWWIN subroutine, which is based on a Kow correlation method described by W. Meylan, P. Howard and R. Boethling in "Improved method for estimating water solubility from octanol/water partition coefficient". *Environ. Toxicol. Chem*. 15:100-106. 1995.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated and measured water solubility data for representative constituents of the Low 1,3-Butadiene C4 Category are listed below. The data identify a potential water solubility range for substances represented by the eight CAS numbers under Test Substance. Substances in this category do not have a specific water solubility value. Actual water solubility ranges of substances in this category will vary dependent on their loading rate (i.e., weight of test material added to a volume of water). Commercial products in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C4. The eight chemicals selected to represent the water solubility range of this category are C4 hydrocarbons that that can be found in substances identified by the eight CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, olefinic process (distillation)

	knowledge, and percentage of the composition of the represented process streams. Substance Constituent / Calculated WS (mg/L @ 25°C) / Measured WS* (mg/L @ 25°C) Isobutane 496.4 175.1 n-butane 424.1 135.6 isobutylene 495.6 399.2 cis-butene-2 652.7 423.5 trans-butene-2 652.7 407.1 butene-1 557.7 354.8 1,2-butadiene 687.8 na 1,3-butadiene 732.4 792.3 * Experimental values from EPIWIN database. na = not available The data represent a potential water solubility range for substances represented by the eight CAS numbers under Test Substance.
Test Substance:	The Low 1,3-Butadiene C4 Category includes the following CAS numbers: 106-97-8 Butane 106-98-9 1-Butene 115-11-7 1-Propene,2-methyl 25167-67-3 Butenes 68477-42-9 Gases, petroleum, extractive, C3-5, butene-isobutylene-rich 68477-83-8 Gases, petroleum, C3-5 olefinic-paraffinic alkylation feed 68527-19-5 Hydrocarbons, C1-4, debutanizer fraction 68606-31-5 Hydrocarbons C3-5, butadiene purification by-product Low 1,3-Butadiene C4 Category substances arise from production processes associated with ethylene manufacturing. The eight CAS numbers are used to describe the seven process streams arising from the ethylene process, associated butadiene purification process and other related C4 processes. Four of these process streams are complex mixtures while the remaining three describe high purity hydrocarbons. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent. With the exception of CAS 106-97-8 (butane) these

	substances contain significant levels of olefins. More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	Based on calculated constituent data, substances in this category can have a water solubility range of 424.1 to 732.4 mg/L @ 25°C. Based on measured constituent data, substances in this category can have a water solubility range of 135.6 to 792.3 mg/L @ 25°C.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential water solubility range for substances represented by the eight CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low 1,3-Butadiene C4 Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for water solubility range based on constituent data.
Reference:	EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA. (Water solubility values were calculated by the WSKOWWIN subroutine and measured data came from the database in the computer program.)
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

ENVIRONMENTAL FATE ROBUST SUMMARIES

Photodegradation (Direct)

Test Substance:	Other TS [CAS # 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5]
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Type (air, soil, water, other):	Water
Light Source:	Not applicable
Light Spectrum: • **Wave length value (upper/lower)**	Not applicable
Relative Intensity:	Not applicable
Test Substance Spectrum:	Not applicable
Test Conditions: • **Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol**	Not applicable

Direct Photolysis: • **Results: half-life, % degradation, quantum yield**	**Summary** In the environment, direct photolysis will not significantly contribute to the degradation of constituent chemicals in the Low 1,3-Butadiene C4 Category (C4 refers to a chemical with 4 carbons). The Low 1,3-Butadiene C4 Category includes seven process streams: • C4 Raffinate 1 • C4 Raffinate 2 • Isobutylene • Butene-1 • C4 Raffinate 3 • Butane • Catalytic butylenes Eight CAS numbers (see Test Substance) identify substances derived from these process streams. As discussed below, the reaction process involved in direct photolysis occurs when sufficient light energy excites a molecule to the degree that a structural transformation occurs. In general, substances in this category do not contain component chemicals that will undergo direct photolysis. **The Low 1,3-Butadiene C4 Category** A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. The process streams in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C4. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent, and with the exception of CAS 106-97-9 (butane), these streams contain significant levels of olefins. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated Low 1,3-Butadiene C4. The typical compositions of the streams in this category are shown in Table 2. The definitions found in the TSCA Chemical Substance Inventory for the CAS numbers included in this group are vague with respect to composition. Therefore, it is possible to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the same stream (composition or process).

	Low 1,3-butadiene streams arise from production processes associated with ethylene manufacturing. More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). The plan is available on the U.S. Environmental Protection Agency website under the HPV Chemical Program. A brief description of the production and composition of the seven process streams in this category are: **C4 Raffinate 1** is a co-product of the butadiene extraction process unit. **C4** Raffinate 1 is the balance of the C4 butadiene concentrate after separation of butadiene by a solvent process, either extraction or more typically extractive distillation. C4 Raffinate 1 consists predominantly of C4 mono-olefins and C4 paraffins. The stream is sometimes referred to as mixed butylenes because the composition is often about 75% C4 mono-olefins. The saturated hydrocarbons in C4 Raffinate 1 are mostly iso- and normal-butane. The mono-olefin content varies depending on the feedstock of the ethylene process unit that produced the C4 butadiene concentrate. • **C4 Raffinate 2** is produced by the further processing of C4 Raffinate 1 to remove the isobutylene. This can be accomplished in a two-step process by reaction with water to make tertiary-butyl alcohol or with methanol to produce methyl-tertiary-butyl-ether, which can be re-cracked to high purity isobutylene. This stream consists predominantly of butene-1, butene-2 and butanes. • **Isobutylene** can be obtained from C4 Raffinate 1 by reaction with water or methanol and then re-cracking the product to high purity isobutylene. Alternatively, isobutylene is obtained by isomerization of Raffinate 2 or by dehydrogenation of isobutane. Typically, commercial isobutylene is 95% pure. • **Butene-1** is produced by distillation from isobutylene plant raffinate. • **C4 Raffinate 3** is the stream that remains after removal of butene-1 from C4 Raffinate 2. It is a mixed butenes product, containing the mixed isomers cis- and trans-butene-2 and sometimes n-butane. • **Butane** is sometimes used as feedstock for the ethylene process. An ethylene producer who operates an isobutylene

alkylation process (typically a petroleum refinery process used to produce alkylates for gasoline formulations) lists butane from this source as a co-product. Butane is also sometimes separated by distillation from C4 Raffinate 3.

- **Catalytic butylenes** refers to the C4 cut from a catalytic cracker (a petroleum refinery process). A typical composition is about 55% butenes and 45% butanes with a carbon number distribution of C3 to C5. The stream is relatively low in 1,3-butadiene and diolefins (e.g. a few tenths of a percent). In some cases the stream is a combination of catalytic cracker C4 butylenes and ethylene process C4 Raffinate 1 from the butadiene unit.

Photolysis of Hydrocarbons

The direct photolysis of an organic molecule occurs when it absorbs sufficient light energy to result in a structural transformation (2). The reaction process is initiated when light energy in a specific wavelength range elevates a molecule to an electronically excited state. However, the excited state is competitive with various deactivation processes that can result in the return of the molecule to a non excited state.

The absorption of light in the ultra violet (UV)-visible range, 110-750 nm, can result in the electronic excitation of an organic molecule. Light in this range contains energy of the same order of magnitude as covalent bond dissociation energies (2). Higher wavelengths (e.g. infrared) result only in vibrational and rotational transitions, which do not tend to produce structural changes to a molecule.

The stratospheric ozone layer prevents UV light of less than 290 nm from reaching the earth's surface. Therefore, only light at wavelengths between 290 and 750 nm can result in photochemical transformations in the environment (2). Although the absorption of UV light in the 290-750 nm range is necessary, it is not always sufficient for a chemical to undergo photochemical degradation. Energy may be re-emitted from an excited molecule by mechanisms other than chemical transformation, resulting in no change to the parent molecule.

A conservative approach to estimating a photochemical degradation rate is to assume that degradation will occur in proportion to the amount of light wavelengths >290 nm absorbed by the molecule (3). Saturated hydrocarbons do not absorb light above 200 nm. Some characteristic absorbance maxima (λ_{max})

	and associated molar absorptivities (ε) for selected unsaturated hydrocarbons are shown below (2): **λ below 290 nm** **λ above 290 nm** Hydrocarbon λ_{max} ε λ_{max} ε Ethylene 193 10,000 - - 1,3-Butadiene 217 2,090 - - Benzene 255 215 - - Olefins with one double bond, or two conjugated double bonds, which constitute the majority of the chemicals in the Low 1,3-Butadiene C4 Category, do not absorb appreciable light energy above 290 nm. The absorption of UV light to cause cis-trans isomerism about the double bond of an olefin occurs only if it is in conjugation with an aromatic ring (2). Substances in the Low 1,3-Butadiene C4 Category do not contain component molecules that will undergo direct photolysis. Therefore, this fate process will not contribute to a measurable degradative removal of chemical components in this category from the environment. **References** 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. Virginia, USA. 2. Harris, J. C. 1982. "Rate of Aqueous Photolysis," Chapter 8 in: W. J. Lyman, W. F. Reehl, and D. H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, USA. 3. Zepp, R. G. and D. M. Cline. 1977. Rates of Direct Photolysis in the Aqueous Environment, Environ. Sci. Technol., 11:359-366.
Indirect Photolysis: • **Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life**	Not applicable

Degradation Products: • **Note: Identification, concentration**	Unknown
Test Substance:	The Low 1,3-Butadiene C4 Category includes the following CAS numbers: 106-97-8 Butane 106-98-9 1-Butene 115-11-7 1-Propene,2-methyl 25167-67-3 Butenes 68477-42-9 Gases, petroleum, extractive, C3-5, butene-isobutylene-rich 68477-83-8 Gases, petroleum, C3-5 olefinic-paraffinic alkylation feed 68527-19-5 Hydrocarbons, C1-4, debutanizer fraction 68606-31-5 Hydrocarbons C3-5, butadiene purification by-product
Conclusion:	Not applicable
Reliability:	These data represent a key study for characterizing the potential of substances in the Low 1,3-Butadiene C4 Category to undergo direct photodegradation.
Reference:	American Chemistry Council, Olefins Panel. 2002. Photodegradation (Direct): Low 1,3-Butadiene C4 Category. Rosslyn, VA, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

Photodegradation (Indirect)

Test Substance:	Other TS [CAS # 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5]
Method/Guideline:	Calculated values using AOPWIN version 1.89, a subroutine of the computer program EPIWIN version 3.04
Year (guideline):	1999
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Type (air, soil, water, other):	Not applicable
Light Source:	Sunlight
Light Spectrum: • **Wave length value (upper/lower)**	Natural sunlight
Relative Intensity:	1
Test Substance Spectrum:	Not applicable
Test Conditions: • **Note: Concentration, temperature, test system type, replication, deviations from guideline or protocol**	Indirect photodegradation, or atmospheric oxidation potential, is based on the structure-activity relationship methods developed by R. Atkinson. Temperature: 25°C Sensitizer: OH radical Concentration of Sensitizer: 1.5 E^6 OH radicals/cm^3
Direct Photolysis: **Results: half-life, % degradation, quantum yield**	Not applicable

Indirect Photolysis: • **Results: type of sensitizer, concentration of sensitizer, rate constant, % degradation, half-life**	**The Low 1,3-Butadiene C4 Category** Low 1,3-Butadiene C4 Category substances arise from production processes associated with ethylene manufacturing. The eight CAS numbers are used to describe the seven process streams arising from the ethylene process, associated butadiene purification process and other related C4 processes. Four of these process streams are complex mixtures while the remaining three describe high purity hydrocarbons. Commercial products in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C4. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent, and with the exception of CAS 106-97-8 (butane), these streams contain significant levels of olefins. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated Low 1,3-Butadiene C4. The eight chemicals selected to represent the atmospheric oxidation potential of this category are C4 hydrocarbons that can be found in substances identified by the eight CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, olefinic process (distillation) knowledge, and percentage of the composition of the represented process streams. **Atmospheric Oxidation of Hydrocarbons** In the environment, organic chemicals emitted into the troposphere are degraded by several important transformation processes. The dominant transformation process for most compounds is the daylight reaction with hydroxyl (OH-) radicals (Atkinson, 1988, 1989). The rate at which an organic compound reacts with OH- radicals is a direct measure of its atmospheric persistence (Meylan and Howard, 1993). AOPWIN estimates the rate constant for the atmospheric, gas-phase reaction between photochemically produced

hydroxyl radicals and organic chemicals. The rate constants estimated by the program are then used to calculate atmospheric half-lives for organic compounds based upon average atmospheric concentrations of hydroxyl radicals.

Since the reactions only take place in the presence of sunlight, the atmospheric half-lives are normalized for a 12-hour day.

Chemical	Calculated* half-life (hrs)	OH- Rate Constant (cm^3/molecule-sec)
Isobutane	52.6	2.4 E^{-12}
n-butane	48.8	2.6 E^{-12}
isobutylene	2.5	51.7 E^{-12}
cis-butene-2	2.3	56.7 E^{-12}
trans-butene-2	2.0	64.3 E^{-12}
butene-1	4.7	27.4 E^{-12}
1,2-butadiene	4.1	31.1 E^{-12}
1,3-butadiene	1.9	66.6 E^{-12}

* Atmospheric half-life values are based on a 12-hr day.

More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (Olefins Panel, 2001).

References

1. Atkinson, R. 1988. Estimation of gas-phase hydroxyl radical rate constants for organic chemicals. *Environ. Toxicol. Chem*. **7**:435-442.
2. Atkinson, R. 1989. Kinetics and mechanisms of the gas-phase reactions of the hydroxyl radical with organic compounds. J. Phys. Chem. Ref. Data Monograph No. 1, Amer. Inst. Physics & Amer. Chem. Soc., NY.
3. Meylan, W.M. and P.H. Howard. 1993. Computer estimation of the atmospheric gas-phase reaction rate of organic compounds with hydroxyl radicals and ozone. *Chemosphere* **12**:2293-2299.
4. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.

Degradation Products: • **Note: Identification, concentration**	Unknown
Test Substance:	The Low 1,3-Butadiene C4 Category includes the following CAS numbers: 106-97-8 Butane 106-98-9 1-Butene 115-11-7 1-Propene,2-methyl 25167-67-3 Butenes 68477-42-9 Gases, petroleum, extractive, C3-5, butene-isobutylene-rich 68477-83-8 Gases, petroleum, C3-5 olefinic-paraffinic alkylation feed 68527-19-5 Hydrocarbons, C1-4, debutanizer fraction 68606-31-5 Hydrocarbons C3-5, butadiene purification by-product
Conclusion:	Atmospheric oxidation via hydroxyl radicals can be a significant route of degradation for products in this category. Based on calculated values, products in this category can have an atmospheric half-life range of 1.9 to 52.6 hours as a result of indirect photolysis by hydroxyl radical attack.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by AOPWIN. The data represent a potential atmospheric half-life range for substances represented by the 8 CAS numbers under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low 1,3-Butadiene C4 Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for atmospheric half-life range based on constituent data.
Reference:	Meylan, M., SRC 1994-1999. AOPWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.

Other (source):	American Chemistry Council, Olefins Panel (Prepared 10/03)

Hydrolysis (Stability in Water)

Test Substance:	Other TS [CAS # 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5]
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
Type (test type):	Not applicable
GLP (Y/N):	Not applicable
Year (study performed):	Not applicable
Analytical Monitoring:	Not applicable
Test Conditions: • **Note: Concentration preparation, vessel type, volume, replication, deviations from guideline or protocol**	Not applicable
Results: **Units/Value:** • **Note: Analytical method, observations, half-lives by pH, degradation products**	Not applicable
Test Substance:	The Low 1,3-Butadiene C4 Category includes the following CAS numbers: 106-97-8 Butane 106-98-9 1-Butene 115-11-7 1-Propene,2-methyl 25167-67-3 Butenes 68477-42-9 Gases, petroleum, extractive, C3-5, butene-isobutylene-rich 68477-83-8 Gases, petroleum, C3-5 olefinic-paraffinic alkylation feed 68527-19-5 Hydrocarbons, C1-4, debutanizer fraction 68606-31-5 Hydrocarbons C3-5, butadiene purification by-product Low 1,3-Butadiene C4 Category products arise from production

	processes associated with ethylene manufacturing. The eight CAS numbers are used to describe the seven process streams arising from the ethylene process, associated butadiene purification process and other related C4 processes. Four of these process streams are complex mixtures while the remaining three describe high purity hydrocarbons. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent. With the exception of CAS 106-97-8 (butane) these products contain significant levels of olefins. More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	**Summary** In the environment, hydrolysis will not contribute to the degradation of chemicals in the Low 1,3-Butadiene C4 Category (C4 refers to a chemical with 4 carbons). This category includes seven process streams: • C4 Raffinate 1 • C4 Raffinate 2 • Isobutylene • Butene-1 • C4 Raffinate 3 • Butane • Catalytic butylenes Eight CAS numbers (see Test Substance) identify substances derived from these process streams. As discussed below, the chemicals in these streams are composed of carbon and hydrogen and are not amenable to hydrolysis because of their molecular structure and the chemical reaction required for this type of transformation to occur. **The Low 1,3-Butadiene C4 Category** A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. The process streams in this category consist of both high purity hydrocarbons and

	complex hydrocarbon reaction products with a carbon number distribution that is predominantly C4. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent, and with the exception of CAS 106-97-9 (butane), these streams contain significant levels of olefins. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated Low 1,3-Butadiene C4. The definitions found in the TSCA Chemical Substance Inventory for the CAS numbers included in this group are vague with respect to composition. Therefore, it is possible to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the same stream (composition or process). Low 1,3-butadiene streams arise from production processes associated with ethylene manufacturing. More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). The plan is available on the U.S. Environmental Protection Agency website under the HPV Chemical Program. A brief description of the production and composition of the seven process streams in this category are: • **C4 Raffinate 1** is a co-product of the butadiene extraction process unit. **C4** Raffinate 1 is the balance of the C4 butadiene concentrate after separation of butadiene by a solvent process, either extraction or more typically extractive distillation. C4 Raffinate 1 consists predominantly of C4 mono-olefins and C4 paraffins. The stream is sometimes referred to as mixed butylenes because the composition is often about 75% C4 mono-olefins. The saturated hydrocarbons in C4 Raffinate 1 are mostly iso- and normal-butane. The mono-olefin content varies depending on the feedstock of the ethylene process unit that produced the C4 butadiene concentrate. • **C4 Raffinate 2** is produced by the further processing of C4 Raffinate 1 to remove the isobutylene. This can be accomplished in a two-step process by reaction with water to make tertiary-butyl alcohol or with methanol to produce methyl-tertiary-butyl-ether, which can be re-cracked to high purity isobutylene. This stream consists predominantly of butene-1, butene-2 and butanes.

- **Isobutylene** can be obtained from C4 Raffinate 1 by reaction with water or methanol and then re-cracking the product to high purity isobutylene. Alternatively, isobutylene is obtained by isomerization of Raffinate 2 or by dehydrogenation of isobutane. Typically, commercial isobutylene is 95% pure.

- **Butene-1** is produced by distillation from isobutylene plant raffinate.

- **C4 Raffinate 3** is the stream that remains after removal of butene-1 from C4 Raffinate 2. It is a mixed butenes product, containing the mixed isomers cis- and trans-butene-2 and sometimes n-butane.

- **Butane** is sometimes used as feedstock for the ethylene process. An ethylene producer who operates an isobutylene alkylation process (typically a petroleum refinery process used to produce alkylates for gasoline formulations) lists butane from this source as a co-product. Butane is also sometimes separated by distillation from C4 Raffinate 3.

- **Catalytic butylenes** refers to the C4 cut from a catalytic cracker (a petroleum refinery process). A typical composition is about 55% butenes and 45% butanes with a carbon number distribution of C3 to C5. The stream is relatively low in 1,3-butadiene and diolefins (e.g. a few tenths of a percent). In some cases the stream is a combination of catalytic cracker C4 butylenes and ethylene process C4 Raffinate 1 from the butadiene unit.

Hydrolysis of Hydrocarbons as a Function of Molecular Structure

Hydrolysis of an organic molecule occurs when a molecule (R-X) reacts with water (H_2O) to form a new carbon-oxygen bond after the carbon-X bond is cleaved (2,3). Mechanistically, this reaction is referred to as a nucleophilic substitution reaction, where X is the leaving group being replaced by the incoming nucleophilic oxygen from the water molecule.

The leaving group, X, must be a molecule other than carbon because for hydrolysis to occur, the R-X bond cannot be a carbon-carbon bond. The carbon atom lacks sufficient electronegativity to be a good leaving group and carbon-carbon

	bonds are too stable (high bond energy) to be cleaved by nucleophilic substitution. Thus, hydrocarbons, including alkenes, are not subject to hydrolysis (3) and this fate process will not contribute to the degradative loss of chemical components in this category from the environment. Under strongly acidic conditions the carbon-carbon double bond found in alkenes, such as those in the Low 1,3-Butadiene C4 Category, will react with water by an addition reaction mechanism (2). The reaction product is an alcohol. This reaction is not considered to be hydrolysis because the carbon-carbon linkage is not cleaved and because the reaction is freely reversible (3). Substances that have a potential to hydrolyze include alkyl halides, amides, carbamates, carboxylic acid esters and lactones, epoxides, phosphate esters, and sulfonic acid esters (4). The substances in the Low 1,3-Butadiene C4 Category are primarily olefins that contain at least one double bond (alkenes). The remaining chemicals are saturated hydrocarbons (alkanes). These two groups of chemicals contain only carbon and hydrogen. As such, their molecular structure is not subject to the hydrolytic mechanism discussed above. Therefore, chemicals in the Low 1,3-Butadiene C4 Category have a very low potential to hydrolyze, and this degradative process will not contribute to their removal in the environment. **References** 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA. 2. Gould, E.S. (1959), Mechanism and Structure in Organic Chemistry, Holt, Reinhart and Winston, New York, NY, USA. 3. Harris, J.C. (1982), "Rate of Hydrolysis," Chapter 7 in: W.J. Lyman, W.F. Reehl, and D.H. Rosenblatt, eds., Handbook of Chemical Property Estimation Methods, McGraw-Hill Book Company, New York, NY, USA. 4. Neely, W. B. 1985. Hydrolysis. In: W. B. Neely and G. E. Blau, eds. Environmental Exposure from Chemicals. Vol I., pp. 157-173. CRC Press, Boca Raton, FL, USA.
Reliability:	Not applicable

Reference:	American Chemistry Council, Olefins Panel. 2002. Hydrolysis: Low 1,3-Butadiene C4 Category. Rosslyn, VA, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

Transport / Distribution (Fugacity)

Test Substance:	Other TS [CAS # 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5]
Method/Guideline:	Calculated according to Mackay Level I, EQC Model version 1.01
Year (guideline):	1997
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Estimation Temperature:	25°C
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment. Physicochemical input values for the model were calculated using the EPIWIN Estimation v 3.04 program (1). Measured input values were also used where available and obtained from the EPIWIN database (1). Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota). 1. EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Calculated partitioning data for representative constituents of the Low 1,3-Butadiene C4 Category are listed below. The data identify a potential distribution for substances represented by the eight CAS numbers under Test Substance. Actual distribution of substances in this category will vary dependent on their constituent composition. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction

products with a carbon number distribution that is predominantly C4. The eight chemicals selected to represent the environmental distribution range of this category are C4 hydrocarbons that are common across the 8 CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, and olefinic process (distillation) knowledge.

The range of distribution data for constituent chemicals in each of the compartments can be used as an estimate of the partitioning behavior for category substances.

The following Mackay Level I model distribution values for representative constituents of substances in this category were determined using physicochemical input data calculated using the EPIWIN program:

	Calculated* Percent Distribution		Measured** Percent Distribution	
Chemical	Air	Water	Air	Water
Isobutane	99.99	0.01	99.99	0.01
n-butane	99.98	0.02	99.99	0.01
isobutylene	99.98	0.02	99.99	0.01
cis-butene-2	99.97	0.03	99.98	0.02
trans-butene-2	99.97	0.03	99.98	0.02
butene-1	99.98	0.02	99.99	0.01
1,2-butadiene	99.96	0.04	99.96	0.04
1,3-butadiene	99.97	0.03	99.97	0.03

* Distribution values determined using calculated input data from EPIWIN program

** Distribution values determined using input data from the EPIWIN program experimental database

Distribution of each chemical to each remaining compartment (soil, sediment, suspended sediment, biota) was calculated as less than 0.01%. Mobility in the environment is expected to be high due to the relatively high water solubility and high vapor pressure of these chemicals.

Test Substance:	The Low 1,3-Butadiene C4 Category includes the following CAS numbers: 106-97-8 Butane 106-98-9 1-Butene 115-11-7 1-Propene,2-methyl 25167-67-3 Butenes 68477-42-9 Gases, petroleum, extractive, C3-5, butene-isobutylene-rich 68477-83-8 Gases, petroleum, C3-5 olefinic-paraffinic alkylation feed 68527-19-5 Hydrocarbons, C1-4, debutanizer fraction 68606-31-5 Hydrocarbons C3-5, butadiene purification by-product
Test Substance: (cont'd)	Low 1,3-Butadiene C4 Category substances arise from production processes associated with ethylene manufacturing. The eight CAS numbers are used to describe the seven process streams arising from the ethylene process, associated butadiene purification process and other related C4 processes. Four of these process streams are complex mixtures while the remaining three describe high purity hydrocarbons. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent. With the exception of CAS 106-97-8 (butane) these substances contain significant levels of olefins. More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	The partitioning data represent a potential distribution range for substances in the eight CAS numbers listed under Test Substance. Substances in the Low 1,3-Butadiene C4 Category are calculated to partition primarily to air with a smaller percentage partitioning to water. Relatively high vapor pressure and high water solubility largely control the partitioning behavior of constituent chemicals in substances

	from this category. The input data used to run the EQC Level I model included estimated values calculated by the EPIWIN program based on chemical structure and measured data from the EPIWIN database. A comparison of the distribution data developed using either all calculated input values or measured values where data were available indicate a similar partitioning behavior and support the use of the dataset for chemicals without any measured data.
Reliability:	(2) Reliable with restrictions The input data used to run the EQC Level I model include calculated and experimental values available through the EPIWIN program. The data represent a potential environmental distribution range for substances with the eight CAS numbers listed under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low 1,3-Butadiene C4 Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for distribution range based on constituent data.
Reference:	Mackay, D.A. DiGuardo, S. Paterson, and C. Cowan. EQC Model Version 1.01. 1997. Available from the Environmental Modeling Centre, Trent University, Canada.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

Biodegradation

Test Substance:	Other TS [CAS # 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5]
Method/Guideline:	Other: Technical discussion
Year (guideline):	Not applicable
Type (test type):	Not applicable
GLP:	Not applicable
Year (study performed):	Not applicable
Inoculum:	Not applicable
Exposure Period:	Not applicable
Test Conditions: • **Note: Concentration prep., vessel type, replication, test conditions.**	Not applicable
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method.**	Not applicable
Test Substance:	The Low 1,3-Butadiene C4 Category includes the following CAS numbers: 106-97-8 Butane 106-98-9 1-Butene 115-11-7 1-Propene,2-methyl 25167-67-3 Butenes 68477-42-9 Gases, petroleum, extractive, C3-5, butene-isobutylene-rich 68477-83-8 Gases, petroleum, C3-5 olefinic-paraffinic alkylation feed 68527-19-5 Hydrocarbons, C1-4, debutanizer fraction 68606-31-5 Hydrocarbons C3-5, butadiene purification by-product

	Low 1,3-Butadiene C4 Category substances arise from production processes associated with ethylene manufacturing. The eight CAS numbers are used to describe the seven process streams arising from the ethylene process, associated butadiene purification process, and other related C4 processes. Four of these process streams are complex mixtures while the remaining three describe high purity hydrocarbons. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent. With the exception of CAS 106-97-8 (butane) these substances contain significant levels of olefins. More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	**SUMMARY** In the environment, biodegradation will not contribute significantly to the loss of chemicals in substances from the Low 1,3-Butadiene C4 category (C4 refers to a chemical with 4 carbons). The Low 1,3-Butadiene C4 category includes seven process streams: • C4 Raffinate 1 • C4 Raffinate 2 • Isobutylene • Butene-1 • C4 Raffinate 3 • Butane • Catalytic Butylenes Eight CAS numbers (see Test Substance) identify substances derived from these process streams. The substances contain various chemicals composed of carbon and hydrogen. As discussed below, substances in this category are gaseous. If they are released to the environment, their chemical components will partition primarily to the air where they can degrade rapidly by physicochemical reactions. It is far less likely that substances from this category will partition to environmental compartments where they could be degraded

by bacteria.

The Low 1,3-Butadiene C4 Category

A process stream is a mixture of chemicals that arises from a chemical reaction or separation activity. The process streams in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C4. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent, and with the exception of CAS 106-97-9 (butane), these streams contain significant levels of olefins. That is why this group is considered a category for purposes of the High Production Volume (HPV) Chemical Program, and designated Low 1,3-Butadiene C4.

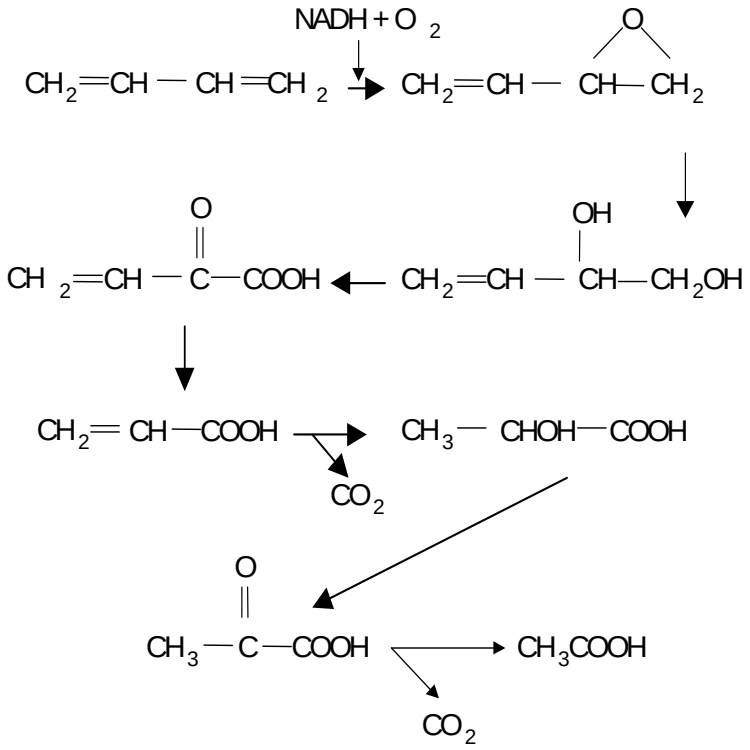
The definitions found in the TSCA Chemical Substance Inventory for the CAS numbers included in this group are vague with respect to composition. Therefore, it is possible to find that the same CAS number is correctly used to describe different streams (compositions) or that two or more different CAS numbers are used to describe the same stream (composition or process).

Low 1,3-butadiene streams arise from production processes associated with ethylene manufacturing. More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). The plan is available on the U.S. Environmental Protection Agency website under the HPV Chemical Program. A brief description of the production and composition of the seven process streams in this category are:

- **C4 Raffinate 1** is a co-product of the butadiene extraction process unit. **C4** Raffinate 1 is the balance of the C4 butadiene concentrate after separation of butadiene by a solvent process, either extraction or more typically extractive distillation. C4 Raffinate 1 consists predominantly of C4 mono-olefins and C4 paraffins. The stream is sometimes referred to as mixed butylenes because the composition is often about 75% C4 mono-olefins. The saturated hydrocarbons in C4 Raffinate 1 are mostly iso- and normal-butane. The mono-olefin content varies depending on the feedstock of the ethylene process

	unit that produced the C4 butadiene concentrate. • **C4 Raffinate 2** is produced by the further processing of C4 Raffinate 1 to remove the isobutylene. This can be accomplished in a two-step process by reaction with water to make tertiary-butyl alcohol or with methanol to produce methyl-tertiary-butyl-ether, which can be re-cracked to high purity isobutylene. This stream consists predominantly of butene-1, butene-2 and butanes. • **Isobutylene** can be obtained from C4 Raffinate 1 by reaction with water or methanol and then re-cracking the product to high purity isobutylene. Alternatively, isobutylene is obtained by isomerization of Raffinate 2 or by dehydrogenation of isobutane. Typically, commercial isobutylene is 95% pure. • **Butene-1** is produced by distillation from isobutylene plant raffinate. • **C4 Raffinate 3** is the stream that remains after removal of butene-1 from C4 Raffinate 2. It is a mixed butenes product, containing the mixed isomers cis- and trans-butene-2 and sometimes n-butane. • **Butane** is sometimes used as feedstock for the ethylene process. An ethylene producer who operates an isobutylene alkylation process (typically a petroleum refinery process used to produce alkylates for gasoline formulations) lists butane from this source as a co-product. Butane is also sometimes separated by distillation from C4 Raffinate 3. • **Catalytic Butylenes** refers to the C4 cut from a catalytic cracker (a petroleum refinery process). A typical composition is about 55% butenes and 45% butanes with a carbon number distribution of C3 to C5. The stream is relatively low in 1,3-butadiene and diolefins (e.g. a few tenths of a percent). In some cases the stream is a combination of catalytic cracker C4 butylenes and ethylene process C4 Raffinate 1 from the butadiene unit. **Biodegradation of Hydrocarbons** Biodegradation is the use of a chemical by microorganisms as a source of energy and carbon. The parent chemical is broken down to simpler, smaller chemicals, which can be converted to inorganic forms such as carbon dioxide, nitrate, sulfate, and water.

	Substances in the Low 1,3-Butadiene C4 Category are gaseous hydrocarbons, composed predominantly of chemicals with carbon numbers smaller than C5. Consequently, their availability to microbial degraders will be significantly limited. Component chemicals from all seven process streams in this category are simple hydrocarbons, the majority of which will partition primarily to the air where physical processes will contribute to their degradation [see the atmospheric oxidation potential (AOP) data (as mediated by hydroxyl radical attack) for specific degradation rates of selected chemicals from this category; AOP data were developed for this category under the HPV Chemical Program]. All chemicals from this category that partition to the air are calculated to degrade rapidly due to physical processes and not persist. Because of the partitioning behavior of chemicals in this category, biodegradative processes will be less likely to contribute to their loss from the environment. Substances from the Low 1,3-Butadiene C4 Category do not lend themselves to being evaluated for biodegradability using standard experimental techniques because of their physical state. However, there is microbial metabolism information for chemicals in this category that demonstrates that they can be biodegraded. Watkinson and Morgan (6) state that microbial metabolism of aliphatic alkenes, such as those in the Low 1,3-Butadiene C4 Category, can be initiated by attack at the double bond. Four degradative processes have been identified: • oxygenase attack upon a terminal methyl group to the corresponding unsaturated alcohol and acid, • subterminal oxygenase attack to the corresponding alcohol and acid, • oxidation across the double bond to the corresponding epoxide, and • oxidation across the double bond to the corresponding diol. Experimental studies to determine a catabolic pathway for 1,3-butadiene as mediated by a *Nocardia* sp. (3), for example, resulted in the following proposed series of reactions:



The intermediary metabolic steps depicted above result in the production of acetic acid, CH3COOH, which can be further metabolized. In addition, 1,3-butadiene has been estimated to have an aerobic aquatic biodegradation half-life ranging from 1 to 4 weeks (2).

The potential biodegradability of some of the other components including butane, 1-butene, and 2-butene has been summarized and metabolic pathways leading to their biodegradation have been described (4, 5). These chemicals have been shown to biodegrade to high extents such that if they were to partition to either a terrestrial or aqueous environment, they would be subject to biodegradative processes that would result in their removal from the environment.

In summary, because the C4 and lighter chemical components of this category will partition to the air, physical degradative processes will dominate their fate. Data show that these chemicals are subject to rapid physical degradation. Chemical components of this category that are greater than C4 also have a potential to partition to the air to a great extent, where they will also degrade rapidly in a

	similar manner. However, they also have a potential to partition to aquatic and terrestrial environments where they are subject to biological processes that can result in their rapid biodegradation. Overall, substances from this category and their component chemicals are expected to degrade rapidly in the environment and not persist. **References** 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. Virginia, USA. 2. Howard, P.H., R.S. Boethling, W.F. Jarvis, W.M. Meylan, and E.M. Michalenko. 1991. Handbook of Environmental Degradation Rates. H.T. Printup Ed. Lewis Publishers, Chelsea, MI, USA. 3. Watkinson, R.J. and H.J. Somerville. 1976. The Microbial Utilization of Butadiene. Shell Research Limited, Sittingbourne Research Centre, Kent, UK. 4. van Agteren, M.H., S. Keuning, and D.B. Janssen. 1998. Handbook on Biodegradation and Biological Treatment of Hazardous Organic Compounds. Kluwer Academic Publishers. Boston, CT, USA. 5. Hartmans, S. 1993. Biodegradation of chlorinated and unsaturated hydrocarbons in relation to biological waste-gas treatment. Thesis Wageningen University. NL. 6. Watkinson, R.J. and P. Morgan. 1990. Physiology of aliphatic hydrocarbon-degrading microorganisms. *Biodegradation*. 1:79-92.
Reliability:	Not applicable
Reference:	American Chemistry Council, Olefins Panel. 2002. Biodegradation: Low 1,3-Butadiene C4 Category. Rosslyn, VA, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

HUMAN HEALTH ROBUST SUMMARIES

Acute Toxicity

Test Substance	Isobutylene 99.4% pure, Purity determined by National Bureau of Standards freezing point method.
Method	
Method/guideline followed	No guideline specified, acceptable scientific method
Type (test type)	Acute effects evaluation
GLP	No
Year	1950
Species/Strain	Dog, strain (or breed) not specified
Sex	Not specified
No. of animals per sex/dose	4 dogs
Vehicle	Air
Route of administration	Inhalation
Test Conditions	This pharmacology study was performed to elucidate relationships between chemical structure and physiological activity. Of particular interest was the ratio of anesthetic to respiratory arrest concentrations (anesthetic index) in the mouse and the specific characteristic of inducing severe arrhythmia/fibrillation in surgically anesthesized dogs after IV injection of epinephrine (method of Meeks *et al*., 1937 and Carr & Krantz, 1949). Dogs were administered each of the 9 test materials including isobutylene, 1- butene or 2-butene,cis, at sufficient dose and duration to induce an appropriate level of anesthesia followed by I.V. administration of epinephrine to produce cardiac stimulation. Reviewer comments: Compounds that can sensitize the heart in this test are believed to be ones that might induce heart irregularities under stressful conditions.
Results	
LC_{50} with confidence limits.	No LC50 was determined. Arrhythmias of different levels of severity were produced with each agent. The arrhythymias were least severe with isobutylene, which produced only mild tachycardia and minor voltage changes after epinephrine injection in all 4 dogs, suggesting a wider margin of safety in exposure conditions.
Remarks	
Conclusions	
(study author)	Irregularities of cardiac rhythm of at least moderate severity were produced with all compounds except isobutylene that caused only

	mild tachycardia and minor voltage changes after epinephrine injection.
Data Quality	
Reliability	2. Reliable with restrictions. This is not a standard acute toxicity study. It is a research study using non-standard methods that were appropriate for the purpose.
References	Virtue, R.W. 1950. Anesthetic Effects in Mice and Dogs of Some Unsaturated Hydrocarbons and Carbon Oxygen Ring Compounds. Pro. Soc. Exp. Biol. Med. 73: 259-262 (See additional acute summary on mouse research) Meek, W.J., Hathaway, H.R. and Orth, O.S. 1937. J. Pharm. Exp. Thera. 61: 240. Carr, C.J. and Krantz, J.C. 1949. Fed. Proc. 8:279.
Other	
Last changed	Revised 2/07/2001 (Prepared by a contractor to the Olefins Panel)

Acute Toxicity

Test Substance	Isobutylene 99.4% pure. Purity determined by Nat'l Bureau of Standards freezing point method.
Method	
Method/guideline followed	No guideline specified, acceptable scientific method
Type (test type)	Acute Effects Evaluation
GLP	No
Year	1950
Species/Strain	Mouse, strain not reported
Sex	Not specified
No. of animals per sex per dose	Approx. 64 mice used to obtain each reported value
Vehicle	Oxygen
Route of administration	Whole body inhalation
Test Conditions	The purpose of this research study was to compare the anesthetic properties of 20 different highly purified unsaturated hydrocarbons and carbon-oxygen ring compounds. Concentrations required for surgical anesthesia and for respiratory arrest were measured. Experiments were carried out in a large stoppered jar equipped with apparatus to introduce known quantities of oxygen (21%) or test compound at 25-27^{0}C under atmospheric pressure. CO2 was absorbed with NaOH. Experiments were limited to concentrations causing anesthesia in 10 min. and were terminated after 20 min. Probit analysis was used to determine conc/effect relationships.
Results	
LC_{50} with confidence limits.	LC50s were not measured. For isobutylene, surgical anesthesia occurred at a concentration of 19.8% and respiratory arrest at 32% giving an anesthetic index of 1.6. Isobutylene demonstrated the widest range between anesthesia and respiratory arrest in this series, suggesting a better margin of safety.
Remarks	
Conclusions	
(study author)	Results support the concept that narcotic potency increases with molecular weight and degree of unsaturation.
Data Quality	
Reliability	2. Reliable with restrictions. This is not a standard acute toxicity study. It is research study using non-standard methods. Mouse strain and sex were not specified. Methods were appropriate for the purpose.

References	Virtue, R.W. 1950. Anesthetic Effects in Mice and Dogs of Some Unsaturated Hydrocarbons and Carbon Oxygen Ring Compounds. Proc. Soc. Exp. Biol. Med 73:259-262. (See additional acute summaries on other mouse and dog research)
Other	
Last changed	Revised 2/07/2001 (Prepared by a contractor to the Olefins Panel)

Genetic Toxicity - *in vitro*

Test Substance	
Test substance	Isobutylene, 99.8% liquefied .
Method	
Method/guideline followed	Comparable to standard bacterial mutation assays
Type	Reverse mutation bacterial
System of testing	Ames Salmonella assay with and without metabolic activation and *E. coli*
GLP	GLP equivalent
Year	1981
Species/Strain	*Salmonella typhimurium* TA1535, TA1537, TA1538, TA100, TA98; *E. coli* WP2uvrA(pKM101)
Metabolic activation	Yes
Species and cell type	Male rat liver
Quantity	50µl S-9 homogenate in 0.5ml S-9mix/plate
Induced or not induced	Aroclor 1254 induced – 500 mg/kg in corn oil, administered 5 days prior to sacrifice
Concentrations tested	1st test: 5, 10, 20, 30, 40, 50%. 2nd test: 10, 20, 40, 60, 80, 100%
Statistical Methods	None employed. Criteria for positive responses were, for TA100 a 1.5 fold increase and for TA1535, TA1537, TA1538, TA98 and E.coli, a doubling of revertant colonies compared to mean negative control values at some dose. Tests were also observed for dose response.
Remarks for Test Conditions	Bacteria were freshly prepared by 16 hour culturing in nutrient broth prior to use and monitored for strain sensitivity. An agar overlay comprised of 2 ml agar, 0.5 ml S-9 mix or phosphate buffer, and 0.1 ml fresh bacteria was mixed and poured on minimal agar plates. When set, plates were inverted, placed in jars of known volume and exposed to isobutylene at 37^0 C for 48 hours, then incubated an additional 24 hours in fresh air. Concentrations of isobutylene were achieved by mixing hydrocarbon-free artificial air and test gas through flow meters before delivery into incubation jars. Flow meters were calibrated by comparing standard registered flow rates with actual flow rates measured by gas burette at atmospheric pressure and ambient temp. Actual flow rates were obtained by multiplying registered air flow rates by the appropriate conversion factor. Approx. 25 liters gas/air filled each 6.25 liter jar during exposure. Actual gas concentrations inside the incubation jars were not measured. Duplicate plates were used in the first trial for each test, only one plate was used at each dose in the repeat trial/test. Negative control: hydrocarbon free artificial air, Positive

	gas control: vinyl chloride 30% in air in TA 1535, TA100 ± S9, Other pos. controls: 4-actyl aminofluorene 1.0 mg/plate in TA1538, TA98 +S9; methyl methane sulfonate 100 µg/plate in *E.coli* –S9, and 9-amino acridine 20 µg/plate in TA1537 -S9.
Results	
Genotoxic effects	No mutagenic activity was induced by isobutylene in any strain at any concentration in the first or second tests. Reduction in number of colonies in all strains indicative of toxicity and growth inhibition was observed with and without metabolic activation at 80% and 100% isobutylene. Positive controls responded appropriately, inducing from 3 fold –30 fold increases above negative controls ±S9.
Conclusions	
(contractor)	Isobutylene was adequately tested at sufficiently high doses to induce toxicity, and is not mutagenic to bacteria in this test system
Data Quality	
Reliabilities	2. Reliable with restrictions. Only 2 plates/dose in initial trial and only 1 plate/dose in repeat trial of each test was used. Gas concentration within chambers was not measured.
Reference	McGregor, D.B., Reach,C.G. 1981. Isobutylene: Ames test for Mutagenic Activity with Salmonella TA 1535, TA100, TA1537, TA1538, TA98, and E.coli WP2 uvrB (pKM101). unpublished Rpt# 2098, IRI Proj. 704338 Inveresk Research Institute, for Essochem Europe, Inc. Machelen, Belgium
Other	
Last changed	Revised 5/15/2001 (Prepared by a contractor to the Olefins Panel)

Genetic Toxicity - *in vitro*

Test Substance	
Test substance	Isobutylene, liquefied, from Essochem Europe, Inc., CAS Number 115-11-7
Method	
Method/guideline followed	Adequate scientific method based on Clive *et al.* (1972, 77, 79), Amacher *et al*. (1979)
Type	Mammalian cell point mutation assay
System of testing	Mouse lymphoma
GLP	Yes
Year	1981
Species/Strain	Mouse lymphoma L5178Y TK^+/TK^- cell line from Clive
Metabolic activation	Yes
Species and cell type	Male Fischer 344 rat liver
Quantity	1 ml S-9/flask (9 parts cofactors:1 part 9000 G liver prep)
Induced or not induced	Aroclor 1254 induced. Administered ip 500 mg/kg, 5 days prior to sacrifice
Concentrations tested	100% or 50, 25, 12.5 , 6.25% isobutylene diluted with 5% CO2 in air
Statistical Methods	None employed. Positive response is defined as a doubling of mutant frequency (mutant colonies ÷ 10^5 survivors) compared to solvent controls with a dose response over two consecutive concentrations. An increase in absolute mutant colonies is highly desirable.
Remarks for Test Conditions	In the preliminary toxicity test, mouse lymphoma cells ($3x10^6$ cells) in culture flasks were exposed to isobutylene at concentrations of 100 – 6.25% without metabolic activation in incubation jars. Concentrations were blended by passing air and isobutylene through flow meters into a mixing chamber, before delivery into the incubation jars. Flow meters were calibrated by comparing standard registered flow rates with actual flow rates measured by gas burette at atmospheric pressure and ambient temperature. Actual flow rates were obtained by multiplying registered flow rates by appropriate conversion factor. Approximately 25 l gas/air mixture was flushed through each 6.25 l jar during exposure. Actual gas concentrations in jars were not measured. Incubation was carried out with shaking for 24 hours at 37^0 C. After incubation, test atmosphere was removed and cells were harvested by centrifugation. Resuspended cells were transferred to fresh tissue culture flasks, gassed with 5% CO2 in air and incubated at 37^0 C. Cell density was measured each day for three days by

	counting with a Neubauer haemocytometer to determine toxicity. In the definitive mutation test, 10 ml of $3x10^6$ exponentially growing L5178Y cells were exposed to isobutylene at concentrations of 100%-6.25% with and without metabolic activation. All cultures were incubated with shaking (150 rpm) at 37^0 C for 24 hours. Positive control compund without S-9 was ethyl methane sulfonate (400, 200 µg/ml); with S-9, 2-acetylamino fluorine (100, 50 µg/ml); cultures were treated for 3 hours. After incubation, cells were harvested by centrifugation, resuspended in fresh medium, and samples from each suspension plated on soft agar for varying times. For day 0 survival, cells were plated immediately after exposure (3 plates/dose level), allowed to set at 4^0 C, equilibrated with 5% CO2/air and incubated at 37^0 C for 10 days. For expression of genetic damage, cells multiplied in liquid medium for 3 days following exposure. On the third day, cell cultures were adjusted to $3x10^5$ cells/ml, diluted in cloning medium, dispensed to 3 plates /dose level and incubated at 37^0 C for 10 days to determine cell survival. For mutant colony selection, cells were dispensed into cloning medium containing 5 µg/ml triflurothymidine (TFT), 3 plates/ dose group, and incubated at 37^0 C for 7-10 days. At the end of incubation, mutant colonies were counted manually.
Results	
Genotoxic effects	Preliminary toxicity results in the absence of S-9 indicated severe toxicity at 100% isobutylene due either to isobutylene itself or prolonged hypoxia to cells caused by exposure to 100% test gas atmosphere. Varying degrees of toxicity also occurred at other doses, only the lowest dose 6.25% was non-toxic. In the first of two mutation tests without S-9, cultures treated with isobutylene induced more TFT resistant colonies than controls but no mutant frequencies reach doubling. Numbers of colonies on survival plates were lower than normal producing overall higher mutant frequencies. These unusual distributions were due to inadequate precleansing of cultures with methotrexate prior to use. In the second experiment, following two additional rounds of cleansing with methotrexate, the number of mutant colonies induced by isobutylene and those in the negative control cultures were much lower and the number of survival colonies much increased. No dose of isobutylene induced a mutant frequency greater than the negative control. Of three experiments performed with S-9, the first was rejected because incubation with S-9 for 24 hours killed 80-90% cells in all cultures including the positive controls, and inadequate cleansing with methotrexate resulted in excess mutant colonies in the negative control group. In the subsequent 2 tests, shorter exposure of 16 hours substantially reduced S-9 induced

	toxicity. Exposure to isobutylene at concentrations up to 100% did not result in any significant increase in mutant colonies compared to negative control (CO2/air) cultures. Positive control treatment produced appropriate increases in mutant frequency.
Conclusions (contractor)	In both the absence and presence of S-9 mix, isobutylene showed no evidence of mutagenic activity in the mouse lymphoma assay.
Data Quality *Reliabilities*	2. Reliable with restrictions. No direct measurement of exposure concentration or analysis of incubation jar atmosphere was performed. Results of these tests are valid and the lack of mutagenic effect was reproducible despite poor initial cell cleansing and toxicity due to initial overexposure to S-9.
Reference	McGregor, D.B., Ross, C.A. 1981. Isobutylene: Assessment of mutagenic potential in the Mouse lymphoma mutation assay. Inveresk Research International, Musselburgh, Scotland for Essochem Europe Inc., Machelen, Belgium. Clive *et al*. 1972. Mut. Res. 77-87; 1977 Handbook of Mutagenicity Test Procedures, Kilbey *et al*. Eds., Elsevier, pp161-173; 1979 Mut. Res. 59: 61-108. Amacher *et al*., 1979. Mut. Res. 64: 391-406.
Other *Last changed*	Revised 2/07/2001 (Prepared by a contractor to the Olefins Panel)

Genetic Toxicity - *in vitro*

Test Substance	
Test substance	Isobutylene, liquefied, from Essochem Europe, Inc., CAS Number 115-11-7
Method	
Method/guideline followed	Adequate scientific method based on Heidelberger
Type	*In vitro* Cell Transformation
System of testing	Mouse embryo fibroblast derived cell line
GLP	Yes
Year	1981
Species/Strain	C3H/10T½ Cl 8 mouse cell line
Metabolic activation	Yes
Species and cell type	Male Fischer 344 Rat liver
Quantity	5% S-9 mix (9 parts cofactor:1 part 9000 G liver prep/flask)
Induced or not induced	Aroclor induced: 500 mg/kg administered ip 5 days prior to sacrifice
Concentrations tested	Prelim. Tox: 100% isobutylene or 50, 25, 12.5 ,6.25% diluted with 5%CO2 in air Transformation assay: 100%, 50, 25% in 5% CO2/air
Statistical Methods	None employed. Positive response is defined as the presence of type II or type III transformed foci in treated cultures with evidence of dose response and reproducibility in repeat assay. Compounds which transform fibroblast cells have a high probability of inducing tumors if injected in immunosuppressed mice.
Remarks for Test Conditions	Preliminary toxicity assay without metabolic activation was performed to establish a range of concentrations for the transformation assay. Five ml. Samples of cells from a culture at density of 200 cells/ml were pipetted into plastic tissue culture flasks, incubated in 5% CO2/air overnight for equilibration, then medium was replaced with fresh medium supplemented with fetal bovine serum (10% v/v). Flasks with caps screwed on lightly were placed in incubation jars which were flushed with 100% isobutylene or isobutylene mixed with 5% CO2/air to achieve concentrations ranging from 50%-6.25%. Concentrations were blended by passing air and isobutylene through flow meters into a mixing chamber, before delivery into the incubation jars. Flow meters were calibrated by comparing standard registered flow rates with actual flow rates measured by gas burette at atmospheric pressure and ambient temperature. Actual flow rates were obtained by multiplying registered flow rates by appropriate conversion

	factor. Approximately 25 l gas/air mixture was flushed through each 6.25 l jar during exposure. Actual gas concentrations in jars were not measured. Jars were sealed and incubated with shaking (50 rpm) at 37^0 C for 24 hours. Exposure medium was then replaced with fresh medium and culture flasks incubated for an additional 3 weeks. Cells were harvested with trypsin and counted for toxicity in Neubauer haemocytometers. For the transformation assay, cultures were treated as above, except that S-9 mix was added to one half flasks (6/dose group) and all flasks (12/dose group) were placed in incubation jars flushed with 100%, 50% or 25% isobutylene. After 24 hours incubation with shaking, medium was changed and cells were incubated in flasks for 8 weeks. Medium was changed twice weekly until cells reached confluence and weekly thereafter. At 8 weeks, cells were fixed in methanol, stained with Giemsa and scored for transformed foci. Positive control chemicals were 3-methylcholanthrene (30, 15 µg/ml), ethyl methane sulfonate (250, 125 µg/ml), 2-acetylaminofluorene (10, 5 µg/ml) and 2-aminoanthracene (5, 2.5 µg/ml). Negative controls were CO2/air, DMSO or acetone.
Results Genotoxic effects	In the preliminary toxicity test without S9, only 100% isobutylene caused cell toxicity either due to isobutylene itself or prolonged hypoxia resulting from exposure to 100% test gas atmosphere. In the transformation assay with or without metabolic activation, no transformed colonies were observed at any exposure level. Positive control compounds, known carcinogens *in vivo*, induced clear evidence of morphological transformation.
Conclusions (contractor)	By criterion used in this laboratory, isobutylene had no transforming effect in C3H/10T½ cells in the presence or absence of liver metabolic activation and is not considered a potential carcinogen *in vivo*.
Data Quality *Reliabilities*	2. Reliable with restrictions. No direct measurement of exposure concentration or analysis of incubation jar atmosphere was performed
Reference	McGregor, D.B., Poole, A. 1981. Isobutylene: Induction of morphological transformation in C3H/10T½ clone 8 cells. Inveresk Research International, Musselburgh, Scotland for Essochem Europe, Inc., Machelen, Belgium

Other *Last changed*	Revised 2/07/2001 (Prepared by a contractor to the Olefins Panel)

Genetic Toxicity - *in vivo*

Test Substance	Isobutylene colorless gas, 100% pure
Remarks	
Method	
Method/guideline followed	Consistent with standard methods. Cites Heddle *et al*. 1983 Report of US EPA GeneTox Program Mut. Res. 123: 61-119 and Cunningham *et al*.1986 Mutagenesis 1: 449-452
Type	Mammalian Bone Marrow Erythrocyte Micronucleus Test
GLP	Yes
Year	1990
Species	Mouse
Strain	B6C3F1
Sex	50 males (10/group)
Route of administration	Whole body Inhalation
Doses/concentration levels	1000, 3260, 10,000 ppm in air; Positive control 1,3-butadiene (1000 ppm)
Exposure period	6 hours/day for 2 days
Statistical methods	Calculation of mean and std. dev. of micronuclei data. Test of equality of group means by standard ANOVA at each time period, followed by Duncan's Multiple Range test if ANOVA was significant. Standard regression used for dose response. Residuals of ANOVA analyzed for normality by Wilk's Criterion.
Remarks for Test Conditions.	Male mice (10/group) were exposed to isobutylene, 6 hours a day for two days at 0, 1000, 3260 or 10,000 ppm. Actual exposure concentrations were determined by on-line gas chromatography reported hourly. Nominal concentrations were calculated. Chamber homogeneity verified by GC in pretrials. All mice were killed 24 hours after second exposure. Bone marrow was removed from both femurs, slides were prepared and stained with acridine orange for fluorescence. 1000 polychromatic erythrocytes (PCEs) were examined for micronuclei. Ratio of PCEs to normochromatic erythrocytes (NCEs) was determined by counting 1000 erythrocytes (PCE + NCE).
Results	
Genotoxic effects NOAEL (NOEL) LOAEL (LOEL)	NOAEL = 10,000 ppm Isobutylene did not induce a statistically significant positive response nor a dose-related increase in the number of micronuclei in PCEs of mouse bone marrow at any dose level. A significant regression coefficient ($p < 0.05$) for increased percentage of PCEs was observed. This event was within historical control values and is not considered biologically significant. Positive control 1,3-

	butadiene induced statistically significant increases in micronuclei and a reduced %PCE indicative of toxicity. Negative control values were within normal range.
Conclusions (study authors)	Isobutylene was not clastogenic in mouse bone marrow under conditions of this test system.
Data Quality *Reliabilities*	1. Reliable without restriction
References	Przygoda, R. 1990. *In vivo* mammalian bone marrow micronucleus assay for isobutylene. Project #236030. Exxon Biomedical Sciences Inc. East Millstone, NJ
Other *Last changed*	2/16/2001 (Prepared by a contractor to the Olefins Panel)

Repeated Dose Toxicity

Test Substance	
Remarks	Isobutylene, 99.7% pure[1], provided by study sponsor
Method	
Method/guideline followed	No guidelines specified, acceptable scientific method
Test type	Subacute toxicity
GLP	Yes
Year	1986
Species	Rat
Strain	Sprague Dawley CD(SR)BR
Route of administration	Oral gavage
Duration of test	4 weeks
Doses/concentration levels	0, 1.49, 14.86, 148.55 mg/kg/day (nominal doses). Test article preparations were considered acceptable with analytical characterizations in the range of 71-134% of nominal conc. Doses were selected based on range-finding study #4298-13-20.
Sex	5 M, 5 F/group
Exposure period	4 weeks
Frequency of treatment	Once/day, 7 days/week
Control group and treatment	5 M, 5 F; corn oil vehicle
Post exposure observation period	None
Statistical methods	Not specified. Group means and std. dev. calculated.
Test Conditions	Groups of rats (5 M,5 F/group, approx. 42 days old at start) received a daily oral dose (5 ml/kg) of corn oil containing various levels of isobutylene, 7 days a week for 4 weeks. Pelleted diet and tap water were available ad lib. Rats were examined twice daily for morbidity and mortality. Body weights were recorded weekly. Blood for hematology and clinical chemistry was collected during week 4. At sacrifice, necropsies were performed and tissues preserved on all rats. Histopathologic evaluations were performed on tissues from all rats in group 1 (corn oil control) and group 4 (High dose)
Results	
NOAEL (NOEL)	NOEL = 14.86 mg/kg/day
LOAEL (LOEL)	LOEL = 148.55 mg/kg/day
Remarks	The only statistically significant treatment related effects were a decrease in total white blood cell count of 11% (M, $p<0.01$) and 44% (F, $p<0.01$) in group 4 rats, predominantly in leucocytes and monocytes. Differential counts of WBC cell types were performed but not analyzed statistically. Slight, non-significant

	increases in BUN (M) and blood glucose (F) in group 4 were also observed. The range finding study (#4298-13/19-20) showed very low levels of isobutylene in blood after dosing with 29.7 mg/kg (nominal) reaching a maximum of 1.2 µg/ml 20 min after dosing, and a maximum of 17% of the dose in the GI tract 20 min after dosing
Conclusions (study authors)	No toxicologically significant changes were observed at dose levels up to 14.86 mg/kg/day administered over 4 weeks. Reviewer comments: A reasonable explanation for the low recovery of isobutylene might be that a considerable amount was lost back to the atmosphere via volatilization after instillation as a bolus dose in the warm stomach.
Quality Reliabilities	2. Reliable with restrictions. Statistical method used was not reported
References	Jones, R.P. 1986. Isobutylene: 4 week oral (gavage) toxicity study in the rat, # 4372-13/21, Hazleton Laboratories Europe Ltd. for Essochem Europe Inc, Machelen, Belgium Jones, R.P. 1986. Isobutylene: Effects of single and repeated oral dosing in the rat (Range finding study) #4298-13/19-20, Hazleton Laboratories Europe Ltd. 1- Isobutylene –preparation and analysis of corn oil formulations: a feasibility study. 1985. #4188-13/7, Hazelton Laboratories Europe Ltd.
Other Last changed	Revised 2/16/2001 (Prepared by a contractor to the Olefins Panel)

Repeated Dose Toxicity

Test Substance	
Remarks	Isobutylene, 99.7% pure, provided by study sponsor
Method	
Method/guideline followed	No guidelines specified, acceptable scientific method
Test type	Inhalation Subchronic
GLP	Yes
Year	1982
Species	Rat
Strain	Sprague Dawley Crl:CD(SR)BR
Route of administration	Whole body inhalation
Duration of test	13 weeks
Doses/concentration levels	0, 250, 1000, 8000 ppm
Sex	10M, 10F/group
Exposure period	13 weeks
Frequency of treatment	6 hours/day, 5 days/week
Control group and treatment	10 M, 10 F; filtered room air exposed
Post exposure observation period	Not applicable
Statistical methods	Analysis performed for the following parameters: body weight, body weight gain, hematology, blood chemistry, organ weights, organ/body wt ratio, organ/brain wt. ratio. Analysis of variance used for normally distributed errors, t-test between control and treatment groups. For non-normal distributions, Kruskal-Wallis test was used; significance determined by the Wilcoxan rank sum test. All tests were two tailed
Test Conditions	Groups of rat (10 M,10 F/group, approx. 47 days old at start) were exposed to isobutylene at 0, 250, 1000, 8000 ppm 6 hrs/day, 5 d/week for 13 wks. Water and pelleted diet were available ad lib. Rats were observed twice daily for morbidity and mortality. Body weight and food consumption were recorded weekly. Fasted blood was collected at initiation, wk 5, and wk 13 for hematology and chemistry. Urine samples were obtained during wk 13 for chemistry. At sacrifice bone marrow was collected, opthalmoscopy and necropsies were performed, and tissues preserved for histopathology.
Results	
NOAEL (NOEL)	NOEL = 8000 ppm
LOAEL (LOEL)	LOEL not determined
Remarks	No biologically significant treatment related effects were observed

	at any dose level. In the intermediate and high dose males and females, elevated ketones were detected in urine (Multistix, semi-quantitative method).
Conclusions (study authors)	No biologically significant treatment related effects were found. The 8000 ppm dose level was the highest that could be tested while ensuring that the chamber concentration would be below the lower explosive limit of isobutylene. Reviewer comments: Toxicological significance of elevated ketones is unknown but the finding indicates absorption of the test article. Possibly urine ketone bodies were derived from metabolism of the 4-carbon isobutylene. It was likely that internal organ exposure was higher in this inhalation study that in the oral studies where ketone bodies were not found (#4298-13/19-20). However, blood and organ levels were not measured after inhalation.
Quality Reliabilities	1. Reliable without restriction
References	Blackett, N.T. 1982. Isobutylene: 13 week inhalation toxicity study in the rat, # 2916-13/11, Hazleton Laboratories Europe Ltd. for Essochem Europe Inc, Machelen, Belgium Jones, R.P. 1986. Isobutylene: Effects of single and repeated oral dosing in the rat (Range finding study) #4298-13/19-20, Hazleton Laboratories Europe Ltd. For Essochem Europe Inc., Machelen, Belgium
Other Last changed	Revised 2/07/2001 (Prepared by a contractor to the Olefins Panel)

Acute Toxicity

Test Substance	1-butene 99.88% pure. Purity determined by National Bureau of Standards mass spectrometry method.
Method	
Method/guideline followed	No guideline specified, acceptable scientific method
Type (test type)	Acute Effects Evaluation
GLP	No
Year	1950
Species/Strain	Mouse, strain not reported
Sex	Not specified
No. of animals per sex per dose	Approx. 64 mice used to obtain each reported value
Vehicle	Oxygen
Route of administration	Whole body inhalation
Test Conditions	The purpose of this research study was to compare the anesthetic properties of 20 different highly purified unsaturated hydrocarbons and carbon-oxygen ring compounds. Concentrations required for surgical anesthesia and for respiratory arrest were measured. Experiments were carried out in a large stoppered jar equipped with apparatus to introduce known quantities of oxygen (21%) or test compound at 25 to 27^0 C under atmospheric pressure. CO2 was absorbed with NaOH. Experiments were limited to concentrations causing anesthesia in 10 min. and were terminated after 20 min. Probit analysis was used to determine conc/effect relationships.
Results	
LC_{50} with confidence limits.	LC50s were not measured. For 1-butene, surgical anesthesia occurred at 22.7% and respiratory arrest at 27.2% giving an anesthetic index of 1.2%.
Remarks	
Conclusions	
(study author)	Results support the concept that narcotic potency increases with molecular weight and degree of unsaturation.
Data Quality	
Reliability	2. Reliable with restrictions. This is not a standard acute toxicity study. It is research study using non-standard methods. Mouse strain and sex were not specified. Methods were appropriate for the purpose.

References	Virtue, R.W. 1950. Anesthetic Effects in Mice and Dogs of Some Unsaturated Hydrocarbons and Carbon Oxygen Ring Compounds. Proc. Soc. Exp. Biol. Med 73:259-262. (See additional acute summaries on other mouse and dog research)
Other	
Last changed	Revised 2/07/2001 (Prepared by a contractor to the Olefins Panel)

Genetic Toxicity - *in vitro*

Test Substance	
Test substance	1-butene, highest purity from Matheson Scientific
Method	
Method/guideline followed	New method validation to evaluate model vapor-phase chemicals for mutagenicity either in solution or by an adsorption/desorption technique.
Type	Reverse mutation bacterial
System of testing	Ames Salmonella assay with or without metabolic activation
GLP	No
Year	1984
Species/Strain	*Salmonella typhimurium* TA97, TA98, TA 100
Metabolic activation	Yes
Species and cell type	Male Sprague Dawley rats or Syrian Golden hamsters
Quantity	500 µl of 5% S9 mix/plate
Induced or not induced	Aroclor 1254-induced at 500 mg/kg, 5 days prior to sacrifice
Concentrations tested	1.3, 4.2, 13.0, 43.2, or 130 µg/plate
Statistical Methods	None reported. Criteria for positive response was increase in revertant colonies at least two-fold background at two increasing dose levels.
Remarks for Test Conditions	1-butene was prepared for biological testing by diffusion into ethanol. Ethanol was placed in a gas washing bottle fitted with a cylinder diffuser. 1-butene was bubbled through the solvent for 10 minutes at 0^0 C. Samples were transferred to Teflon –capped vials and delivered for Ames testing. Aliquots were removed for GC/FID analysis and comparison with standard samples of undiluted 1-butene. The highest mutagenicity test dose was limited by solubility of 1-butene in ethanol to 130 µg/plate. Test sample at 100 µl was introduced to a preincubation mixture containing 100 µl of log-phase bacteria, 500 µl of 5% S9 mix or buffer solution for non-activated tests, and 600 µl of overlay agar per plate which completely filled each vial allowing no headspace. Mixtures were incubated at 37^0 C for 10 minutes without shaking. Contents of vials were equally distributed on 3 plates/dose level and incubated at 37^0 C for 48 hours. Positive control compounds were sodium azide (TA100), 9-aminoacridine (TA97), 2-nitrofluorene (TA98) for non-activated tests, and 2-aminoanthracene for all S9 assays.
Results	
Genotoxic effects	1-butene did not induce increases in revertant colonies at any dose level up to 130µg/plate in any strain of Salmonella tested with or

	without metabolic activation
Conclusions (contractor)	1-butene is not a bacterial mutagen in this test system
Data Quality *Reliabilities*	2. Reliable with restrictions. Study performed to develop new methods to deliver ambient air vapors to bacterial test systems. Study was performed according to standard procedures for the Ames assay with analytical characterization of test compounds. GLPs were not cited.
Reference	Claxton, L.D. 1984. Validation of Chemical and Biological Techniques for Evaluation of Vapors in Ambient Air/Mutagenicity Testing of Twelve (12) Vapor-Phase Compounds. EPA Health Research Lab., Research Triangle Park, NC. EPA-600/1-84-005. Contract # 68-02-3170-082
Other *Last changed*	Revised 2/16/2001 (Prepared by a contractor to the Olefins Panel)

Genetic Toxicity - *in vitro*

Test Substance	
Test substance	1-butene CAS# 106-98-9 supplied by Tokyo Kasei Co. Ltd.
Method	
Method/guideline followed	New method employs gas sampling bag exposure of 1,3 butadiene and 14 additional gases for *in vitro* mutagenicity testing
Type	Reverse mutation bacterial
System of testing	Ames bacterial assay with and without metabolic activation and *E. coli*
GLP	No
Year	1994
Species/Strain	*Salmonella typhimurium* TA98, TA100, TA1535, TA1537; *E. coli* WP2 uvrA
Metabolic activation	Yes
Species and cell type	Sprague Dawley rat liver
Quantity	100 µl S9 homogenate in 0.5 ml S-9 mix/plate
Induced or not induced	Induced with phenobarbitol and 5,6-benzoflavone (dosage and treatment not specified)
Concentrations tested	500 ml exposure vol./plate, max. 50% gas concentration. Gases diluted with HEPA filtered air.
Statistical Methods	None used
Remarks for Test Conditions	Test substance was collected from a cylinder into a 20 liter gas sampling bag. A separate gas bag was filled with a fixed amount of dilution gas (HEPA filtered air). A fixed volume of the test gas was pumped into the dilution bag and mixed. Concentration was calculated by the volume of both the test gas and the dilution air. Characterization of undiluted test gas and samples of diluted gas from the mixed gas bag were performed by GC/FID. Standard exposure conditions were: bacterial plates made by agar overlay method using 2 ml top agar/plate, 100 µl S9 homogenate, or phosphate buffer, 0.1 ml bacteria. Bacterial strains were prepared fresh by preincubating for 10 hours prior to use. When agar overlay was set, plates were placed separately, upside-down without lids in a plate holder and placed in a 10 liter gas sampling bag. The bag was closed and sealed with adhesive tape and air was evacuated. The bag was then filled with diluted 1-butene at an adjusted concentration at a fixed amount per plate (4 plates/dose) and incubated for 24 hours at 37^0 C. At termination of exposure, sterile air was pumped in to replace test atmosphere; plates were removed and allowed to stand in a safety cabinet for 30 min to evaporate all residual gas. Lids were replaced on the plates which

	were incubated for 24 hours at 37^0 C.
Results Genotoxic effects	1-butene did not induce mutagenic events in any strain in this assay with or without metabolic activation. Only maximum dose was reported (50% conc.) and no specific revertant data were supplied for non-mutagenic gases
Conclusions (contractor)	1-butene was not mutagenic in this test system employing a gas sampling bag exposure method. Positive results for 1,3-butadiene and 7 other gaseous compounds confirm the acceptability of this method.
Data Quality *Reliabilities*	2. Reliable with restrictions Specific data for non-mutagenic gases is limited; control values, dose ranges and revertant data are not reported. Data for positive mutagens are more complete and conform to published results
Reference	Araki, A., Noguchi, T., Kato, F., and Matsushima, T. 1994. Improved method for mutagenicity testing of gaseous compounds using a gas sampling bag. Mut. Res. 307: 335-344. (See separate summary for data on 2-butene)
Other *Last changed*	Revised 2/16/2001 (Prepared by a contractor to the Olefins Panel)

Genetic Toxicity - *in vivo*

Test Substance	1-butene, colorless gas with slight aromatic odor. Stability and purity data referred to study sponsor.
Remarks	
Method	Comparable to standard micronucleus assays, cites Salamone, MF (1983) in Chemical Mutagens vol. 8. Eds. De Serres & Hollaender, Plenum Press NY
Method/guideline followed	
Type	Mammalian Bone Marrow Erythrocyte Micronucleus Test
GLP	Yes
Year	1985
Species	Mouse
Strain	Crl:CDR(IRC)Br Swiss
Sex	Male and female; pretest 2 M, 2 F/group: full study 10 M, 10 F/group & one group of 15 M, 15 F
Route of administration	Whole body inhalation
Doses/concentration levels	Pretest 1000, 9000, 18,000 ppm; full study 1000, 9000, 22,000 ppm
Exposure period	2 hours/day for 2 days: one group received 22,000 ppm 2 hrs/day for 1 day
Statistical methods	Values from treated groups for daily mean body weights, group means and std. dev. for polychromatic erythrocytes (PCEs) with micronuclei (MN) , and group mean ratios of PCE to normochromatic erythrocytes (NORMs) were calculated and compared with vehicle control values by Student's t-test. Positive response was indicated by statistically significant ($p<0.05$) increases in micronucleated PCE at any dose level with a dose related response evident. Results were considered equivocal if only one of these criteria was met.
Remarks for Test Conditions.	1-butene was premixed with ambient air and introduced into inhalation chambers containing groups of mice (10 M,10 F) at concentrations of 0, 1000, 9000,or 22,000 ppm 2 hrs/day for 2 days. One half of each group was killed on day 3 and the remainder on day 4 following exposure. One group (15 M, 15 F) exposed for one day to 22,000 ppm was killed on days 2, 3, 4 after treatment (5/sex/day) Test concentrations were monitored each day by gas chromatography. Positive control mice given cyclophosphamide (75 mg/kg) ip daily for 2 days were killed on day 3. Slides of bone marrow smears were prepared, stained with May-Grunewald/Giemsa stain and examined microscopically. For each mouse, 1000 PCE and all mature erythrocytes (NORMs) were counted. Data collected included group mean body weights for each day, total PCEs, total NORMs, PCEs with MN, and NORMs

	with MN.
Results	
Genotoxic effects NOAEL (NOEL) LOAEL (LOEL)	Mice at all doses were unconscious during exposure to 1-butene but recovered when exposure ended. No other clinical signs were observed and no mortality occurred at any dose level. Inhalation of 1-butene by mice did not induce significant changes in micronucleus formation in PCEs or NORMs and did not cause significant changes in the ratio of PCE/NCE. NOAEL = 22,000 ppm
Conclusions	
(study authors)	1-butene given by inhalation 2 hrs/day for 2 days to mice had no effect on the frequency of micronucleated erythrocytes in bone marrow. Under these test conditions, 1-butene does not induce chromosome damage.
Data Quality	
Reliabilities	1. Reliable without restriction. Study conforms to standard design. GLP have been followed and final QA statement is included in the report.
References	Khan, S.H. Ward, C.O. 1985. Micronucleus test of Gulftene® 4. Unpublished report # 84-2113 by Gulf Life Sciences Center for Gulf Oil Chemicals Co
Other	
Last changed	2/16/2001 (Prepared by a contractor to the Olefins Panel)

Acute Toxicity

Test Substance	2-butene,cis 96.18% pure. Purity determined by Nat'l Bureau of Standards freezing point method.
Method	
Method/guideline followed	No guideline specified, acceptable scientific method
Type (test type)	Acute Effects Evaluation
GLP	No
Year	1950
Species/Strain	Mouse, strain not reported
Sex	not specified
No. of animals per sex per dose	approx 64 mice used to obtain each reported value
Vehicle	oxygen
Route of administration	whole body inhalation
Test Conditions	The purpose of this research study was to compare the anesthetic properties of 20 different highly purified unsaturated hydrocarbons and carbon-oxygen ring compounds. Concentrations required for surgical anesthesia and for respiratory arrest were measured. Experiments were carried out in a large stoppered jar equipped with apparatus to introduce known quantities of oxygen (21%) or test compound at 25-27^0 C under atmospheric pressure. CO2 was absorbed with NaOH. Experiments were limited to concentrations causing anesthesia in 10 min. and were terminated after 20 min. Probit analysis was used to determine conc/effect relationships.
Results	
LC_{50} with confidence limits.	LC50s were not measured. For 2-butene cis, surgical anesthesia occurred at 17.2%, and respiratory arrest at 25.5% giving an anesthetic index of 1.5.
Remarks	
Conclusions	
(study author)	Results support the concept that narcotic potency increases with molecular weight and degree of unsaturation.
Data Quality	
Reliability	2. Reliable with restrictions. This is not a standard acute toxicity study. It is research study using non-standard methods. Mouse strain and sex were not specified. Methods were appropriate for the purpose.

References	Virtue, R.W. 1950. Anesthetic Effects in Mice and Dogs of Some Unsaturated Hydrocarbons and Carbon Oxygen Ring Compounds. Proc. Soc. Exp. Biol. Med 73:259-262. (See additional acute summaries on other mouse and dog research)
Other	
Last changed	Revised 2/07/2001 (Prepared by a contractor to the Olefins Panel)

Acute Toxicity

Test Substance	2-butene, trans 98.92% pure. Purity determined by Nat'l Bureau of Standards freezing point method.
Method	
Method/guideline followed	No guideline specified, acceptable scientific method
Type (test type)	Acute Effects Evaluation
GLP	No
Year	1950
Species/Strain	Mouse, strain not reported
Sex	not specified
No. of animals per sex per dose	Approx. 64 mice used to obtain each reported value
Vehicle	Oxygen
Route of administration	Whole body inhalation
Test Conditions	The purpose of this research study was to compare the anesthetic properties of 20 different highly purified unsaturated hydrocarbons and carbon-oxygen ring compounds. Concentrations required for surgical anesthesia and for respiratory arrest were measured. Experiments were carried out in a large stoppered jar equipped with apparatus to introduce known quantities of oxygen (21%) or test compound at 25-27^0 C under atmospheric pressure. CO2 was absorbed with NaOH. Experiments were limited to concentrations causing anesthesia in 10 min. and were terminated after 20 min. Probit analysis was used to determine conc/effect relationships.
Results	
LC_{50} with confidence limits.	LC50s were not measured. For 2-butene, trans, surgical anesthesia occurred at 18.7%, and respiratory arrest at 21.0% giving an anesthetic index of 1.1.
Remarks	
Conclusions	
(study author)	Results support the concept that narcotic potency increases with molecular weight and degree of unsaturation.
Data Quality	
Reliability	2. Reliable with restrictions. This is not a standard acute toxicity study. It is research study using non-standard methods. Mouse strain and sex were not specified. Methods were appropriate for the purpose.
References	Virtue, R.W. 1950. Anesthetic Effects in Mice and Dogs of Some

	Unsaturated Hydrocarbons and Carbon Oxygen Ring Compounds. Proc. Soc. Exp. Biol. Med 73:259-262. (See additional acute summaries on other mouse and dog research)
Other	
Last changed	Revised 2/07/2001 (Prepared by a contractor to the Olefins Panel)

Acute Toxicity

Test Substance	Butene-2 (42.4% cis, 55.3% trans)
Method	
Method/guideline followed	OECD guideline 403 (1981)
Type (test type)	Acute (limit test)
GLP	Yes
Year	1992
Species/Strain	Rat: Wistar [Crl:WI(WU)BR]
Sex	Males and females
No.of animals per sex per dose	5
Vehicle	Filtered air
Route of administration	Inhalation (whole body)
Test Conditions	During exposure, rats were housed individually in wire mesh stainless steel cages within the inhalation chamber (Hazleton Systems Inc, H1000) at a mean temperature of 23.1^0 C and 49% relative humidity. Chamber concentrations of test article were monitored with a total carbon analyzer (FID) calibrated by passing known atmospheres containing test article over the FID. Rats were exposed for 4 hrs to a test article vapor concentration of 23.1 g/m^3 (actual, approx. 10,000 ppm). After exposure, rats were removed from the chambers and returned to their individual living cages for 14 days of observation; the animal room was maintained at 21.5-23^0 C with relative humidity of 38-67% and a 12 hr light/dark cycle. Diet and water were available ad lib. Body weight was measured before study initiation and at post-dose days 7 and 14. Rats were observed for clinical signs during exposure, shortly after, and once daily during the observation period. After the observation period, rats were sacrificed, necropsied, and examined for gross pathological changes.
Results	
LC_{50} with confidence limits.	LOEL not determined NOEL = 23.1 g/m^3 (approximately 10,000 ppm)
Remarks	Restlessness was observed periodically during and after exposure; no clinical signs were seen during the 14 day observation period. Normal growth also occurred during the observation period. No abnormalities were observed at gross necropsy.
Conclusions	
(study author)	From the results of the present study, it was concluded that the 4-hr

	LC50 value of butene-2 was higher than 23.1g/m^3.
Data Quality Reliability	1. Reliable without restrictions.
References	Arts, J.H.E. 1992. Acute (4-hour) inhalation toxicity study of butene-2 in rats. Report No. V92.183/352130. TNO Nutrition and Food Research, Zeist, The Netherlands.
Other *Last changed*	5/15/2001 (Prepared by a contractor to the Olefins Panel)

Genetic Toxicity - *in vitro*

Test Substance	
Test substance	2-butene CAS# 107-01-7 supplied by Tokyo Kasei Co. Ltd.
Method	
Method/guideline followed	New method employs gas sampling bag exposure of 1,3 butadiene and 14 additional gases for *in vitro* mutagenicity testing
Type	Reverse mutation bacterial
System of testing	Ames bacterial assay with and without metabolic activation and *E. coli*
GLP	No
Year	1994
Species/Strain	*Salmonella typhimurium* TA98, TA100, TA1535, TA1537; *E. coli* WP2 uvrA
Metabolic activation	Yes
Species and cell type	Sprague Dawley rat liver
Quantity	100 µl S9 homogenate in 0.5 ml S-9 mix/plate
Induced or not induced	Induced with phenobarbitol and 5,6-benzoflavone (dosage and treatment not specified)
Concentrations tested	500 ml exposure vol./plate, max. 50% gas concentration. Gases diluted with HEPA filtered air.
Statistical Methods	None used
Remarks for Test Conditions	Test substance was collected from a cylinder into a 20 liter gas sampling bag. A separate gas bag was filled with a fixed amount of dilution gas (HEPA filtered air). A fixed volume of the test gas was pumped into the dilution bag and mixed. Concentration was calculated by the volume of both the test gas and the dilution air. Characterization of undiluted test gas and samples of diluted gas from the mixed gas bag were performed by GC/FID. Standard exposure conditions were: bacterial plates made by agar overlay method using 2 ml top agar/plate, 100 µl S9 or phosphate buffer, 0.1 ml bacteria. Bacterial strains were prepared fresh by preincubating for 10 hours prior to use. When agar overlay was set, plates were placed separately, upside-down without lids in a plate holder and placed in a 10 liter gas sampling bag. The bag was closed and sealed with adhesive tape and air was evacuated. The bag was then filled with diluted 2-butene at an adjusted concentration at a fixed amount per plate (4 plates/dose) and incubated for 24 hours at 37^0 C. At termination of exposure, sterile air was pumped in to replace test atmosphere; plates were removed and allowed to stand in a safety cabinet for 30 min to evaporate all residual gas. Lids were replaced on the plates which were

	incubated for 24 hours at 37^0 C.
Results Genotoxic effects	2-butene did not induce mutagenic events in any strain in this assay with or without metabolic activation. Only maximum dose was reported (50% conc.) and no specific revertant data were supplied for non-mutagenic gases
Conclusions (contractor)	2-butene was not mutagenic in this test system employing a gas sampling bag exposure method. Positive results for 1,3-butadiene and 7 other gaseous compounds confirm the acceptability of this method.
Data Quality *Reliabilities*	2. Reliable with restrictions Specific data for non-mutagenic gases is limited; control values, dose ranges and revertant data are not reported. Data for positive mutagens are more complete and conform to published results
Reference	Araki, A., Noguchi, T., Kato, F., and Matsushima, T. 1994. Improved method for mutagenicity testing of gaseous compounds using a gas sampling bag. Mut. Res. 307: 335-344. (See separate summary for data on 1-butene)
Other *Last changed*	Revised 2/16/2001 (Prepared by a contractor to the Olefins Panel)

Genetic Toxicity - *in vitro*

Test Substance	
Test substance	Butene-2 (42.4% cis, 55.3% trans) from Union Carbide Industrial Gases. Certificate of analysis from supplier.
Method	
Method/guideline followed	OECD Guideline #471 (1981), Method B14 of Commission Directive 84/449/EEC
Type	Reverse mutation in bacteria
System of testing	*Salmonella typhimurium* with and without metabolic activation
GLP	Yes
Year	1992
Species/Strain	*Salmonella typhimurium* TA 1535, TA1537, TA98, TA 100
Metabolic activation	Yes
Species and cell type	Sprague Dawley male rat liver (S9 fraction)
Quantity	10% S9 fraction in S9 mix, (0.05 ml S9 fraction/plate)
Induced or not induced	Aroclor 1254 induced; 500mg/kg single ip injection 5 days before sacrifice
Concentrations tested	0.0, 10, 20, 40, 60, 80%
Statistical Methods	Dunnett's method of linear regression
Remarks for Test Conditions	A 0.1 ml aliquot of Salmonella, 2.0 ml molten top agar, 0.5 ml S9 mix or 0.5 ml pH 7.4 phosphate buffer were mixed in a test tube and poured on minimal agar plates (3 plates/ conc./± S9 mix). Atmospheres of varying concentrations were generated by mixing Butene-2 with clean dry air, using precalibrated gas flow meters as gas flow indicators. Mixtures passed into 10L stainless steel containers holding Salmonella plates with triple vented lids. Concentrations were selected based on a preliminary range finding test with TA100 ± S9; dose-related reduction in frequency of revertant colonies and reduced growth of background lawn observed at 80, 100%. Containers holding 3 stacks of 8 plates each were flushed with appropriate concentrations of butene-2 for 5 min to allow system to equilibrate; containers were incubated at 37^0 C for 48 hrs and number of revertant colonies counted. Analytical determinations were performed by GC on syringe samples of test atmospheres at representative concentrations. Positive control compounds were: -S9, N-ethyl-N' nitro-N-nitrosoguanidine, 3 µg/plate for TA100, 5 µg/plate for TA1535; 9 amino acridine, 80 µg/plate for TA1537; 4-Nitroquinoline-1-oxide, 0.2 µg/plate for TA98; +S9, 2-aminoanthracene 2 µg/plate for TA1535; benzo(a)pyrene 5 µg/plate for all other strains. Vinyl chloride 50% conc. was gaseous positive control for all strains; negative control was clean dry air. The complete experiment was repeated using

	fresh bacteria cultures, test material and control solutions. Criteria for positive response were induction of dose-related and statistically significant increases in mutation rate in one or more strain of bacteria ± S9 in both experiments at subtoxic doses.
Results	
Genotoxic effects	Toxicity was exhibited in all strains at 80% butene-2. In experiment 2, slight toxicity also occurred at 60%. No significant increases in number of revertant colonies of any strain of bacteria were observed at any dose concentration ± S9. Controls performed appropriately
Conclusions	
(contractor)	Butene-2 was not mutagenic in the *Salmonella typhimurium* assay with or without metabolic activation
Data Quality	
Reliabilities	1. Reliable without restrictions
Reference	Thompson, P.W. 1992. Butene-2: Reverse mutation assay "Ames test" using *Salmonella typhimurium*. Proj. #44/812. SafePharm Laboratories, UK, Derby UK.
Other	
Last changed	3/17/2001 (Prepared by a contractor to the Olefins Panel)

Genetic Toxicity - *in vitro*

Test Substance	Butene-2 (42.4% cis, 55.3% trans) from Union Carbide Industrial Gases. Certificate of analysis from supplier.
Test substance	
Method	
Method/guideline followed	OECD Guideline 473 (1981), Method B10 of Commission Directive 84/449/EEC
Type	Chromosome aberrations in mammalian cells.
System of testing	Metaphase analysis in primary blood lymphocyte cultures
GLP	Yes
Year	1992
Species/Strain	Rat – Sprague Dawley (CD-1) males, ages 8-20 wks. from Charles River UK
Metabolic activation	Yes
Species and cell type	Sprague Dawley male rat liver (S9 fraction)
Quantity	20% S9 fraction in S9 mix, (10% v/v S-9 mix/flask)
Induced or not induced	Aroclor 1254 induced; 500 mg/kg single ip injection 5 days before sacrifice
Concentrations tested	0.0, 10, 20, 40, 50, 60, 80, 100%
Statistical Methods	Frequency of cells with aberrations (± gaps) and frequency of polyploid cells (duplicate culture data pooled) were compared with concurrent vehicle control using Fisher's Exact Test UKEMS, Statistical Evaluation of Mutagenicity Test Data (1989).
Remarks for Test Conditions	Atmospheres of varying concentrations were generated by mixing Butene-2 with clean dry air, using precalibrated gas flow meters as gas flow indicators. Mixtures passed through culture flasks for sufficient time (time not specified) to allow equilibration of the system. Analytical determinations were performed by GC on syringe samples of test atmospheres at representative concentrations. Blood samples were drawn from male rats; cells were grown in RPMI medium supplemented with 10% fetal calf serum, 25 mM Hepes and antibiotics, at 37^0 C in a humidified atmosphere of 5% CO2 in air. Duplicate cultures were incubated for 48 hrs, then transferred to tubes, centrifuged and culture medium drawn off and saved. Cells were resuspended in flasks, in fresh culture medium with or without S9 metabolic activation mix and exposed to appropriate concentrations of butene-2 or control materials. Flasks were sealed and shaken to maximize cell exposure for 4 hrs +S9 or 20 hrs -S9. Cells exposed to butene-2 + S9 were resuspended after 4 hrs in original culture medium; one group was harvested at 20 hrs (16 hr recovery), the other at 30 hrs (26 hr recovery) after initiation of treatment; -S9 cultures were

	harvested after 20 full hrs exposure to butene-2. Positive controls were ethyl methyl sulfonate (500 µg/ml) –S9, cyclophosphamide (4.2 µg/ml) +S9; gaseous control was vinyl chloride (50%) in 20 hr group –S9 and 30 hr group +S9. Negative control was clean, dry air.
Results	
Genotoxic effects	Butene-2 caused hemolysis in +S9 cultures at concentrations of 50% and above. In –S9 cultures, 80 and 100% concentrations caused cultures to turn dark brown but return to normal red color by cell harvest. Butene-2 induced steep dose-related decreases in mitotic indices ± S9; especially toxic to lymphocytes at 80% in +S9 20 hr harvest group. However, butene-2 did not induce significant dose-related increases in frequency of structural chromosome aberrations or polyploid cells at any concentration level at any harvest period ± S9. Control compounds performed appropriately.
Conclusions	
(contractor)	Butene-2 produced no significant increases in frequency of chromosome aberrations either in the presence or absence of a liver enzyme metabolizing system. Butene-2 is not clastogenic to rat lymphocytes *in vitro*.
Data Quality	
Reliabilities	1. Reliable without restrictions
Reference	Wright, N.P. 1992. Butene-2: Metaphase analysis in rat lymphocytes *in vitro*. Proj. #44/813. SafePharm Laboratories, UK, Derby UK.
Other	
Last changed	5/15/2001 (Prepared by a contractor to the Olefins Panel)

Repeated Dose Toxicity

Test Substance	
Remarks	Butene-2 (cis and trans ≥95%), mol. wt 56.1, from UCAR Specialty Gases, The Netherlands. Certificate of analysis provided by the supplier
Method	
Method/guideline followed	OECD guideline 422 (draft 1992, final 1996) Combined repeated dose toxicity and reproductive/developmental toxicity test. Used in SIDS
Test type	Subchronic toxicity
GLP	Yes
Year	1992
Species	Rats
Strain	Wistar (Hsd/Cpd:WU) from Charles River, Sulzfeld, F.R.G.; 13 wks old at study initiation
Route of administration	Whole body inhalation
Duration of test	39 to 46 days
Doses/concentration levels	0, 2500, 5000 ppm
Sex	Males and females (12 M, 12 F/group)
Exposure period	Males: 39 to 46 days; Females: pre-mating, mating through Gestation day 19
Frequency of treatment	6 hr/day, 7 days/wk
Control group and treatment	12 M, 12 F; filtered air-conditioned air, 6 hr/day, 7 days/wk
Post exposure observation period	None
Statistical methods	Clinical findings and pathological changes evaluated Fisher's exact probability test. Body wt and food consumption analyzed by one-way anlaysis of variance (ANOVA) followed by Dunnett's multiple comparison test.
Test Conditions	Male and female rats (avg. wt. 299.4 g males, 204.0 g females at study initiation) were assigned to one of three groups by computer randomization based on body weight, and uniquely identified by ear tattoo. During the entire exposure period, animals were housed individually in stainless steel cages within modified multitiered Hazleton 1000 inhalation chambers. Temperature range of 20 to 23^0 C, and relative humidity of 37 to 80% were monitored continuously using thermo-hygrometers with approximately 10 air changes/hour. Lighting in the animal room and Hazleton chamber was 12 hr light/dark cycle. Animals received food and water ad lib except for ½ hr prior to and during exposure. Animals were exposed to a continuous supply of fresh test atmosphere, passed from a cylinder via a pressure reducer,

	stainless steel tubing and 2 calibrated mass flow controllers and rotameters to the inlet at the top of the inhalation chamber (2.2 m^3 capacity), where it was diluted with filtered air-conditioned air to appropriate concentration, directed downward to the animal cages, and eventually exhausted out at the bottom of the chamber. Control rats were exposed to filtered air only. Air flow was monitored by an anemometer and recorded three times/exposure day, providing 11 to 12 air changes/hr. Concentrations of test material were determined with a total carbon analyzer using FID, twice/hr. in each test atmosphere by sampling at locations close to the animal cages. Uniform distribution of butene-2 vapor was verified during preliminary experiments. Nominal concentrations were calculated by mean amount of test material used/hr. divided by mean hourly volume of air passed through the exposure chamber. Top dose level of 5000 ppm was chosen because the estimated body burden was approx. 1000 mg/kg/day, the limit dose for teratology studies in OECD protocol 414. After 2 wks pre-mating exposure, males and females were caged together (1:1) until mating had occurred or one week. Mated females were exposed through day 19 of gestation; males and females that did not mate (1 in control group) were exposed until necropsy at the end of the study. However, data from non-pregnant females was not presented. At terminal necropsy, blood was collected from all parental (F0) animals (males and dams) for hematology and clinical chemistry. Organs were excised and weighed (liver, kidney, thymus, lung, testes, epididymides) and 15 organs/tissues processed for microscopic examination: nose, lungs with trachea and larynx, spleen, heart, brain, seminal vesicles, ovaries (after counting corpora lutea), uterus (after counting implantation sites), any abnormal growths or lesions. All organs in the 5000 ppm and control groups were examined by a pathologist.
Results	
NOAEL (NOEL)	NOAEL(systemic) = 2500 ppm (based on body wt changes)
LOAEL (LOEL)	
Remarks	Mean actual concentration of butene-2 in test atmospheres was 0, 2476 ± 68ppm (5.7 g/m^3) and 5009 ± 88 ppm (11.5 g/m^3). No mortality or treatment-related clinical signs were observed in parental (F0) animals. Male body wt were comparable in all groups but mean body wt change was statistically significantly lower in the 1st and 4th wk of exposure for 2500 ppm group and in the 1st wk of exposure for 5000 ppm group. Female rats showed statistically significantly decreased mean body wt compared to controls at 14 days from start of exposure in 2500 ppm group and at 7 and 14 days of exposure in 5000 ppm group. During gestation, all body weights were comparable in treated and control groups; on lactation day 1, body wt of 5000 ppm dams was

	statistically significantly decreased. Body wt changes in dams were comparable to control throughout the study. Food consumption in males was comparable to controls; food consumption by 5000 ppm females was decreased during the first wk of exposure. No other food consumption differences occurred during the study. In hematology data, the total white blood cell count and number of lymphocytes were increased in male rats in both exposure groups compared to concurrent controls, however there was no dose response, values were within historical control range and concurrent control values were low. No changes were observed in % distribution of white blood cells, any red blood cell parameters, or clotting potential. in males or pregnant females of either exposure group. In clinical chemistry data, plasma calcium concentration was slightly decreased in high-dose males but was not considered toxicologically significant since there was no accompanying change in inorganic phosphate levels. No other treatment-related differences were observed. Mean absolute organ wt and relative wt were comparable in all groups. No abnormal, treatment-related macroscopic changes (all groups) or pathological changes (control and 5000 ppm groups) were observed.
Conclusions (study authors)	Exposure to Butene-2 at concentrations up to 5000ppm did not induce significant systemic toxicity in male rats exposed for 39 to 46 days, or in pregnant female rats exposed for 2 weeks pre-mating, through mating and gestation to day 19.
Quality Reliabilities	1. Reliable without restriction
References	Waalkens-Brendsen, D.H. and Arts, J.H.E. 1992. Combined short term inhalation and reproductive/developmental toxicity screening test with Butene-2 in rats. Proj. #B91-8336 (Study #1410) (see separate summary for reproductive toxicity data)
Other Last changed	5/15/2001 (Prepared by a contractor to the Olefins Panel)

Repeated Dose Toxicity

Test Article	
Remarks	1-BUTENE Purity: ≥99% CAS number: 106-98-9
Method	
Method/guideline followed	OECD 422
Test type	Combined repeated exposure toxicity, reproduction and neurotoxicity screening in rats via whole-body inhalation exposures.
GLP	Yes.
Year	2003
Species	Rat
Strain	Crl:CD® (Sprague-Dawley) IGS BR
Route of administration	Inhalation (gas).
Duration of test	28 days
Doses/concentration levels	0, 500, 2000, or 8000 ppm
Sex	12 males, 12 females per dose group for main study group
Exposure period	6 hours/day.
Frequency of treatment	7 days/week
Control group and treatment	12 males, 12 females, air-only exposed.
Post exposure observation period	Not applicable.
Statistical methods	Mean values of all exposure groups were compared to the mean value for the control group at each time interval. For all parameters except for organ weights, the standard one-way analysis of variance (ANOVA) using the F ratio to assess significance was used. If significant differences among the means were indicated, additional testing was performed using Dunnett's t-test to determine which means were significantly different from the control. Organ weight data was analyzed only by parametric methods. Bartlett's test was performed to determine if groups had equal variances. The standard one-way analysis of variance (ANOVA) using the F ratio to assess significance was used. If significant differences among the means were indicated, additional tests were used to determine which means were significantly different from the control: Dunnett's t-test for homogeneous data, or Cochran and Cox's modified t-test for non-homogeneous data. All t-tests were conducted at the 5% and 1% significance levels. Motor Activity Data was analyzed using split-plot repeated measures ANOVA with model terms for group, animal within group, interval and group by interval interaction. If the group x

	interval interaction was statistically significant (p=0.05), indicating non-parallelism in the behavioral profile between groups, a separate one-way ANOVA for group effects was performed at each interval. If the response data passed on the parallel hypothesis, an ANOVA (using summed responses over intervals) was used to test for the overall treatment effect which constituted the level hypothesis. If any significant overall treatment group effect was found by any of the above ANOVAs, Dunnett's t-test was used to find groups that differed from control. Analyses were performed for sexes separately and combined. Treatment group effects were deemed significant at the p=0.05 level. Plots, tables, listings, and analyses were generated using SAS® version 6.12 for WINDOWS. Analyses were conducted by CATO Research, 200 Westpark Corporate Center, 4364 South Alston Avenue, Durham, NC 27713-2280. The Testing Facility was responsible for the GLP compliance of this subcontractor.
Test Conditions	Groups of 12 male and 12 female Sprague Dawley rats (approximately 8 weeks old) were exposed to the test article as a gas daily by inhalation for approximately six hours/day at exposure levels of 0, 500, 2000, or 8000 ppm. The main study (repeated-exposure general toxicity and neurotoxicity endpoints) males and females were exposed for 28 days, respectively. Effects on general toxicity, neurobehavioral activity, clinical chemistry, coagulation and hematology were evaluated. In addition, a gross necropsy with extensive histopathologic examination of tissues was conducted. The study also contained reproductive and developmental toxicity satellite groups (summarized separately).
Results	
NOAEL (NOEL)	8000 ppm
LOAEL (LOEL)	Not applicable
Remarks	The mean (± standard deviation) analytical (GC) concentrations for the control and the exposure groups were as follows: 0 ± 0, 524 ± 40, 2062 ± 126, and 8271 ± 683 ppm. The analytically measured exposure levels of the airborne test article were reasonably close to the targeted exposure levels. Chamber environmental conditions averaged 23°C temperature and 57% relative humidity. Mean particle size distribution measurements for the exposure indicated that the atmospheres were gas only, as expected, since there was no substantial difference between the test article chambers and the Air Control chambers.

	There was no effect of treatment on survival. All animals survived until the termination of the study. The test animals were unremarkable during the exposure periods (in-chamber) and during non-exposure periods. There were no exposure-related differences in body weights or weight changes or feed consumption in the test article exposed animals compared to the Air Control animals. There was no apparent exposure-related effect on motor activity or function observational battery parameters for either sex in this study. There were no exposure-related differences in hematology or coagulation values or clinical chemistry values in test article exposed animals compared to the Air Control animals at the terminal interval. There were no exposure-related differences in macroscopic postmortem evaluations or organ weights in the test article exposed animals compared to the Air Control animals. There were no microscopic findings considered to be related to exposure to 1-Butene. In comparison with controls, there was a slightly increased incidence and severity of mixed inflammatory cells in the cecal mucosa of rats exposed to 1-Butene at exposure levels of 2000 ppm and above. The cecal mucosa normally contains a small population of mixed inflammatory cells, which acts as a natural defense mechanism against ingested substances or organisms. Increased numbers of inflammatory cells are sometimes seen as a normal spontaneous finding, and this was evident in a few males and females from the control group in this study. Since the finding was present in the control group and there was no clear exposure level response relationship in the treated groups, the increased incidence is considered to be fortuitous and unlikely to be related to treatment with 1-Butene. Other microscopic findings occurred sporadically or showed a similar incidence in control and 1-Butene-treated animals. None were considered to be associated with exposure to the test article.
Conclusions	Exposure of male and female rats to target concentrations of 500, 2000 and 8000 ppm of 1-Butene resulted in no general systemic effects or effects on reproductive performance. Therefore, a no observed effect level (NOEL) of 8000 ppm was determined.
Data Quality Reliabilities	Klimisch value = 1 (Reliable without restrictions).
References	Hoffman G.M. (2003). 1-Butene: A combined repeated

	exposure toxicity, reproduction and neurotoxicity screening in rats via whole-body inhalation exposures. Report of Huntingdon Life Sciences conducted for the American Chemistry Council Olefins Panel. Report reference: 02-4224
Other Last changed	21 May 2003 Robust summary prepared by contractor to Olefins Panel

Toxicity to Reproduction

Test Substance	
Remarks	Butene-2 (cis and trans ≥95%), mol. wt 56.1, from UCAR Specialty Gases, The Netherlands. Certificate of analysis provided by the supplier
Method	
Method/guideline followed	OECD guideline 422 (draft 1992, final 1996) Combined repeated dose toxicity and reproductive/developmental toxicity test. Used in SIDS
Test type	Reproductive/Developmental toxicity screening test
GLP	Yes
Year	1992
Species	Rats
Strain	Wistar (Hsd/Cpd:WU) from Charles River, Sulzfeld, F.R.G.; 13 wks old at study initiation
Route of administration	Whole body inhalation
Duration of test	39 to 46 days
Concentration levels	0, 2500, 5000 ppm
Sex	Males and females (12 M,12 F/group)
Exposure period	Males: 39 to 46 days; Females: pre-mating, mating through Gestation day 19
Frequency of treatment	6 hr/day, 7 days/wk
Control group and treatment	12 M, 12 F; filtered air-conditioned air, 6 hr/day, 7 days/wk
Statistical methods	Fisher's exact probability test for parametric data; Kruskal-Wallis analysis of variance followed by Mann-Whitney U-test for non-parametric data. Analysis of variance followed by Dunnet's multiple comparison tests for body weights and food consumption.
Remarks for Test Conditions.	Male and female rats (avg. wt. 299.4 g males, 204.0 g females at study initiation) were assigned to one of three groups by computer randomization based on body weight, and uniquely identified by ear tattoo. During the entire exposure period, animals were housed individually in stainless steel cages within modified multitiered Hazleton 1000 inhalation chambers. Temperature range of 20 to 23^0 C, and relative humidity of 37 to 80% were monitored continuously using thermo-hygrometers with approximately 10 air changes/hour. Lighting in the animal room and Hazleton chamber was 12 hr light/dark cycle. Animals received food and water ad lib except for ½ hr prior to and during exposure. Animals were exposed to a continuous supply of fresh test atmosphere, passed from a cylinder via a pressure reducer, stainless steel tubing and 2 calibrated mass flow controllers and

	rotameters to the inlet at the top of the inhalation chamber (2.2 m^3 capacity), where it was diluted with filtered air-conditioned air to appropriate concentration, directed downward to the animal cages, and eventually exhausted out at the bottom of the chamber. Control rats were exposed to filtered air only. Air flow was monitored by an anemometer and recorded three times/exposure day, providing 11 to 12 air changes/hr. Concentrations of test material were determined with a total carbon analyzer using FID, twice/hr in each test atmosphere by sampling at locations close to the animal cages. Uniform distribution of butene-2 vapor was verified during preliminary experiments. Nominal concentrations were calculated by mean amount of test material used/hr divided by mean hourly volume of air passed through the exposure chamber. Top dose level of 5000 ppm was chosen because the estimated body burden was approx. 1000 mg/kg/day, the limit dose for teratology studies in OECD protocol 414. After 2 wks pre-mating exposure, males and females were caged together (1:1) until mating had occurred or for 1 wk. Mating was verified by a vaginal plug or sperm in a vaginal smear = Gestation day (GD) 0. Pregnant females were exposed through GD19; after which they were removed from the inhalation chambers and housed individually in the animal room, allowed to litter normally and to rear pups to day 4 of lactation, when both dams and pups were killed. Males, and females that did not mate (1 in control group), were housed individually in chambers and exposed until necropsy at the end of the study. Each rat was observed twice a day for reaction to treatment, ill health or mortality. Body wt of males were recorded weekly; body wt of all females were recorded weekly during pre-mating, mated females on GD0, 7, 14, 21, and on lactation days 1, 4. Food consumption was measured weekly for all rats pre-mating and for males after the mating period ended until study termination; for pregnant females, food consumption was recorded weekly during gestation and days 1 to 4 of lactation. Total litter size and number of pups of each sex, number of stillbirths, grossly malformed pups, if any, and pup body wt were recorded on day 1 and 4 postpartum. Necropsies were performed on stillborns and pups dying during lactation. Macroscopic examinations were performed on these pups and all pups killed on day 4 post-partum, and any abnormalities were recorded. Blood was collected from all parental (F0) animals (males and dams) at terminal necropsy for hematology and clinical chemistry analyses in the subchronic portion of this study. All F0 males and dams were examined macroscopically. Organs were excised and weighed, and tissues processed for microscopic examination. Pregnancies were verified by counting of implantation sites at necropsy; corpora lutea were counted in ovaries prior to fixation.

	Systemic data from non-pregnant females were not reported.
Results NOAEL	NOAEL(reproductive) = 5000 ppm Mean actual concentration of butene-2 in test atmospheres was 0, 2476 ± 68 ppm (5.7 g/m^3) and 5009 ± 88 ppm (11.5 g/m^3). No mortality or treatment-related clinical signs were observed in parental (F0) animals. Male body wt were comparable in all groups but mean body wt change was statistically significantly lower in the 1st and 4th wk of exposure for 2500 ppm group and in the 1st wk of exposure for 5000 ppm group. Female rats showed statistically significantly decreased mean body wt compared to controls at 14 days from start of exposure in 2500 ppm group and at 7 and 14 days of exposure in 5000 ppm group. During gestation, all body weights were comparable in treated and control groups; on lactation day 1, body wt of 5000 ppm dams was statistically significantly decreased. Body wt changes in dams were comparable to control throughout the study. Food consumption in males was comparable to controls; food consumption by 5000 ppm females was decreased during the first wk of exposure. No other food consumption differences occurred during the study. Mating was successful in 11/12 females in the control group and all females 12/12 in each treated group; precoital times were comparable. Female fecundity index was 73% (8/12), 75% (9/12), 83% (10/12) in control, 2500 ppm and 5000 ppm groups, respectively. Duration of pregnancy was comparable in all groups. One high dose female delivered 1 stillborn pup and 12 live pups; all other dams in all groups delivered live pups. Gestation and live birth indices were approx. 100% in all groups. No treatment-related increase in pre-implantation loss occurred. Post-implantation loss was slightly increased in 5000 ppm group but was within historical control limits and the number of implantation sites in the control group was low. Total number of live births in exposed groups was slightly higher than controls. In the control and 2500 ppm groups, one pup died between days 1 and 4 of lactation, viability index was 97 to 100%; sex ratio of pups was similar in all groups. Mean body weight of pups was slightly but not statistically significantly lower in 2500 and 5000 ppm groups, which might be explained by the higher number of pups in these groups compared to controls. No treatment related effects were noted in pups during lactation or at necropsy.
Conclusions (study authors)	Exposure to butene-2 by inhalation during 2 weeks pre-mating, during mating and the gestation period up to and including day 19

	for females, and exposure of males for the entire study (39 to 46 days) did not induce treatment-related reproductive or developmental toxicity.
Data Quality	
Reliabilities	1. Reliable without restriction
References	Waalkens-Brendsen, D.H. and Arts, J.H.E. 1992. Combined short term inhalation and reproductive/developmental toxicity screening test with Butene-2 in rats. Proj. #B91-8336 (Study #1410) (see separate summary for repeat dose toxicity data)
Other	
Last changed	5/15/2001 (Prepared by a contractor to the Olefins Panel)

Developmental Toxicity

Test Substance	Isobutene
Species	rat
Strain	Wistar
Route of admin.	Other: vapor exposure
Exposure period	17 days (day 5 to 21 of gestation)
Frequency of treatm.	6 hours/day
Duration of test	21 days
Doses	500, 2000 and 8000 ppm
Control group	yes, concurrent no treatment
Method	OECD Guideline 414 "Teratogenicity"
Year	2002
GLP	yes
Method	Maternal body weight was evaluated by analysis of covariance. Maternal food cunsumption, the numbers of implantations and live foetuses per female, gravid uterus weight, litter weight, mean foetal weights per litter, and mean manus and pes scores per litter were evaluated by analysis of variance. Pre-implantation loss, post-implantation loss, early intra-uterine deaths, late intra-uterine deaths, major external/visceral defects, minor external/visceral defects, external/visceral variants, major skeletal defects, minor skeletal defects, and skeletal variants were analysed as the proportion of fetuses with each individual manus and pes score, and the proportion of foetuses and the proportion of litters affected with each defect using FISHER'S EXACT test.

Result	Exposure to isobutylene on days 5 to 21 (inclusive) of gestation did not elicit any maternal effects, i.e., there were no treatment-related changes in clinical condition, no effects on maternal body weight or food consumption and no macroscopic findings in tissues examined post mortem. There was no effect of isobutylene on the number, growth or survival of the fetuses in utero. There was no effect of isobutylene on fetal development. Although cleft sternebrae were observed only in fetuses in the isobutylene groups, the incidence of fetuses affected was small and not dose-related and there were no minor changes in the appearance or ossification of the sternebrae to indicate that this area of the skeleton was adversely affected by isobutylene. Also, there was no evidence for an adverse effect of isobutylene on other ossification centres of the skeleton. Isolated differences from control were considered to be incidental. Thus isobutylene at exposure concentrations of up to 8000 ppm is considered not to have any adverse effect on fetal development.
Test Condition	Twenty-four mated female Wistar rats per test group were exposed (whole-body) to dynamic atmospheres of isobutylene for 6 hours per day on days 5 through day 21 (inclusive) of gestation. The target concentrations were 500, 2000 and 8000 ppm. A concurrent control group was exposed to clean air. Chamber concentrations were determined analytically using a gas chromatographic method. Clinical observations were recorded for each animal at least once a day throughout the study (days 1-22 of gestation). On exposure days clinical observation was performed before, during and after exposure. Food consumption, water consumption and body weight of the animals was frequently determined. On day 22 of gestation, all animals were sacrificed and assessed by gross pathology (including weight determinations of the unopened uterus and the placentae). For each dam, corpora lutea were counted and number and distribution of implantation sites (differentiated as resorptions, live and dead fetuses) was determined. The fetuses were removed from the uterus, sexed, weighed and further investigated for any external findings. Thereafter, all fetuses were examined internally for visceral variation and abnormality, sexed and eviscerated. The fetuses were then fixed in 70% industrial methylated spirits. After approximately 24 hours, the head of each fetus was cut along the fronto-parietal suture line and the brain was examined for macroscopic abnormalities. The fetuses were then returned to the 70% methylated spirits, processed and stained with Alizarin Red S and Alcian Blue and then examined for variation and abnormality of bone and cartilage and the degree of ossification of the manus and pes was assessed.

Conclusion	Under the conditions of this prenatal developmental toxicity study, the inhalation exposure of pregnant Wistar rats to isobutylene on days 5 to 21 (inclusive) of gestation elicited no maternal toxicity at all tested concentrations up to 8,000 ppm. There was no effect of isobutylene on the number, growth or survival of the fetuses in utero and no effect on fetal development.
Reliability	(1) valid without restriction
Reference	Central Toxicology Laboratory (CTL) (2002). Isobutylene: Prenatal Developmental Toxicity Study in the Rat. CTL/RR0907/Regulatory Report. Cheshire, UK.

AQUATIC TOXICITY ROBUST SUMMARIES

Fish Acute Toxicity

Test Substance:	Other TS [CAS # 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5]
Method/Guideline:	Other: ECOSAR Computer Model
Year (guideline):	1999
Type (test type):	Acute Fish Toxicity Calculation; LC50
GLP:	Not applicable
Year (study performed):	Not applicable
Species:	Freshwater Fish (calculated toxicity values are not species specific)
Analytical Monitoring:	Not applicable
Exposure Period:	96 hours
Statistical Method:	Not applicable
Test Conditions: • **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**	Log K_{ow} (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The K_{ow} calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental K_{ow} values (EXPKOW.DB). Calculated and measured log K_{ow} data, for representative constituents of the Low 1,3-Butadiene C4 Category, are listed below. Substance Constituent / Calculated log K_{ow} / Measured* log K_{ow} Isobutane: 2.23 / 2.76 n-Butane: 2.31 / 2.89 Isobutylene: 2.23 / 2.34 cis-Butene-2: 2.09 / 2.31 trans-Butene-2: 2.09 / 2.33 Butene-1: 2.17 / 2.40 1,2-Butadiene: 2.06 / na 1,3-Butadiene: 2.03 / 1.99

	na = not available * Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values. 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92. 2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**	Calculated fish acute toxicity values for the eight chemicals representative of substances in the Low 1,3-Butadiene C4 Category are listed below. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C4. The eight chemicals selected to represent the acute toxicity range of this category are C4 hydrocarbons that can be found in substances identified by the eight CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, olefinic process (distillation) knowledge, and percentage of the composition of the represented process streams. The range of toxicity data for substance constituents is an estimate of the potential toxicity of category products. Substance Constituent / Calculated log K_{ow} / Fish Acute 96-hr LC50 (mg/L) Isobutane: 2.23; 26.19 n-Butane: 2.31; 22.03 Isobutylene: 2.23; 25.28 cis-Butene-2: 2.09; 34.23 trans-Butene-2: 2.09; 34.23 Butene-1: 2.17; 28.79 1,2-Butadiene: 2.06; 35.22 1,3-Butadiene: 2.03; 37.59

	Substance Constituent / Measured* log K_{ow} / Fish Acute 96-hr LC50 (mg/L) Isobutane 2.76 8.32 n-Butane 2.89 6.28 Isobutylene 2.34 19.93 cis-Butene-2 2.31 21.26 trans-Butene-2 2.33 20.36 Butene-1 2.40 17.50 1,2-Butadiene na na 1,3-Butadiene 1.99 40.98 na = not available * Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values. The data represent a potential acute toxicity range for substances represented by the eight CAS numbers under Test Substance.
Test Substance:	The Low 1,3-Butadiene C4 Category includes the following CAS numbers: 106-97-8 Butane 106-98-9 1-Butene 115-11-7 1-Propene,2-methyl 25167-67-3 Butenes 68477-42-9 Gases, petroleum, extractive, C3-5, butene-isobutylene-rich 68477-83-8 Gases, petroleum, C3-5 olefinic-paraffinic alkylation feed 68527-19-5 Hydrocarbons, C1-4, debutanizer fraction 68606-31-5 Hydrocarbons C3-5, butadiene purification by-product Low 1,3-Butadiene C4 Category substances arise from production processes associated with ethylene manufacturing. The eight CAS numbers are used to describe the seven process streams arising from the ethylene process, associated butadiene purification process and other related C4 processes. Four of these process streams are complex mixtures while the remaining three describe high purity

	hydrocarbons. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent. With the exception of CAS 106-97-8 (butane) these substances contain significant levels of olefins. More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	Based on the calculated K_{ow} values, substances in this category are expected to have a fish 96-hour LC50 range of 22.03 to 37.59 mg/L. Based on the measured K_{ow} values, substances in this category are expected to have a fish 96-hour LC50 range of 6.28 to 40.98 mg/L.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential acute toxicity range for substances with the eight CAS numbers listed under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low 1,3-Butadiene C4 Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for a range of acute toxicity to fish based on constituent data.
Reference:	Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

Daphnid Acute Toxicity

Test Substance:	Other TS [CAS # 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5]
Method/Guideline:	Other: ECOSAR Computer Model
Year (guideline):	1999
Type (test type):	Acute Daphnid Toxicity Calculation; LC50
GLP:	Not applicable
Year (study performed):	Not applicable
Species:	Daphnid (calculated toxicity values are not species specific)
Analytical Monitoring:	Not applicable
Exposure Period:	48 hours
Statistical Method:	Not applicable
Test Conditions: • **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**	Log K_{ow} (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The K_{ow} calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental K_{ow} values (EXPKOW.DB). Calculated and measured log K_{ow} data, for representative constituents of the Low 1,3-Butadiene C4 Category, are listed below. Substance Constituent — Calculated log K_{ow} — Measured* log K_{ow} Isobutane — 2.23 — 2.76 n-Butane — 2.31 — 2.89 Isobutylene — 2.23 — 2.34 cis-Butene-2 — 2.09 — 2.31 trans-Butene-2 — 2.09 — 2.33 Butene-1 — 2.17 — 2.40 1,2-Butadiene — 2.06 — na 1,3-Butadiene — 2.03 — 1.99 na = not available

Test Conditions: (cont'd) • **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**	* Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values.. 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92. 2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**	Calculated daphnid acute toxicity values for the eight chemicals representative of substances in the Low 1,3-Butadiene C4 Category are listed below. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C4. The eight chemicals selected to represent the acute toxicity range of this category are C4 hydrocarbons that can be found in substances identified by the eight CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, olefinic process (distillation) knowledge, and percentage of the composition of the represented process streams. The range of toxicity data for substance constituents is an estimate of the potential toxicity of category products. Substance Constituent — Calculated log K_{ow} — Daphnid Acute 48-hr LC50 (mg/L) Isobutane — 2.23 — 28.51 n-Butane — 2.31 — 24.11 Isobutylene — 2.23 — 27.53 cis-Butene-2 — 2.09 — 36.91 trans-Butene-2 — 2.09 — 36.91 Butene-1 — 2.17 — 31.21 1,2-Butadiene — 2.06 — 37.89 1,3-Butadiene — 2.03 — 40.27

	Substance Constituent / Measured* log K_{ow} / Daphnid Acute 48-hr LC50 (mg/L) Isobutane 2.76 9.39 n-Butane 2.89 7.15 Isobutylene 2.34 21.86 cis-Butene-2 2.31 23.28 trans-Butene-2 2.33 22.32 Butene-1 2.40 19.28 1,2-Butadiene na na 1,3-Butadiene 1.99 43.88 na = not available * Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values. The data represent a potential acute toxicity range for substances represented by the eight CAS numbers under Test Substance.
Test Substance:	The Low 1,3-Butadiene C4 Category includes the following CAS numbers: 106-97-8 Butane 106-98-9 1-Butene 115-11-7 1-Propene,2-methyl 25167-67-3 Butenes 68477-42-9 Gases, petroleum, extractive, C3-5, butene-isobutylene-rich 68477-83-8 Gases, petroleum, C3-5 olefinic-paraffinic alkylation feed 68527-19-5 Hydrocarbons, C1-4, debutanizer fraction 68606-31-5 Hydrocarbons C3-5, butadiene purification by-product Low 1,3-Butadiene C4 Category substances arise from production processes associated with ethylene manufacturing. The eight CAS numbers are used to describe the seven process streams arising from the ethylene process, associated butadiene purification process and other related C4 processes. Four of these process streams are complex mixtures while the remaining three describe high purity hydrocarbons. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five

	percent. With the exception of CAS 106-97-8 (butane) these substances contain significant levels of olefins. More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	Based on the calculated K_{ow} values, substances in this category are expected to have a daphnid 48-hour LC50 range of 24.11 to 40.27 mg/L. Based on the measured K_{ow} values, substances in this category are expected to have a daphnid 48-hour LC50 range of 7.15 to 43.88 mg/L.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential acute toxicity range for substances with the eight CAS numbers listed under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low 1,3-Butadiene C4 Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for a range of acute toxicity to aquatic invertebrates based on constituent data.
Reference:	Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)

Alga Toxicity

Test Substance:	Other TS [CAS # 106-97-8; 106-98-9; 115-11-7; 25167-67-3; 68477-42-9; 68477-83-8; 68527-19-5; 68606-31-5]
Method/Guideline:	Other: ECOSAR Computer Model
Year (guideline):	1999
Type (test type):	Green Alga Toxicity Calculation; EC50
GLP:	Not applicable
Year (study performed):	Not applicable
Species:	Freshwater Green Alga (calculated toxicity values are not species specific)
Analytical Monitoring:	Not applicable
Exposure Period:	96 hours
Statistical Method:	Not applicable
Test Conditions: • **Note: Concentration prep., vessel type, volume, replication, water quality parameters, environmental conditions, organisms supplier, age, size, weight, loading.**	Log K_{ow} (octanol/water partition coefficient) values and a chemical structure are needed to calculate aquatic toxicity using the ECOSAR model. The K_{ow} calculation is performed by KOWWIN based on an atom/fragment contribution method of Meylan and Howard (1), which is a subroutine in the EPIWIN computer model (2). KOWWIN also has a database of experimental K_{ow} values (EXPKOW.DB). Calculated and measured log K_{ow} data, for representative constituents of the Low 1,3-Butadiene C4 Category, are listed below. Substance Constituent / Calculated log K_{ow} / Measured* log K_{ow} Isobutane: 2.23 / 2.76 n-Butane: 2.31 / 2.89 Isobutylene: 2.23 / 2.34 cis-Butene-2: 2.09 / 2.31 trans-Butene-2: 2.09 / 2.33 Butene-1: 2.17 / 2.40 1,2-Butadiene: 2.06 / na 1,3-Butadiene: 2.03 / 1.99

	na = not available * Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values. 1. Meylan, W. and P. Howard. 1995. Atom/fragment contribution method for estimating octanol-water partition coefficients. J. Pharm. Sci. 84:83-92. 2. Meylan, M., SRC 1994-1999. KOWWIN is contained in the computer program EPIWIN. 1999. Estimation Program Interface for Windows, version 3.04. Syracuse Research Corporation, Syracuse, NY, USA.
Results: **Units/Value:** • **Note: Deviations from protocol or guideline, analytical method, biological observations, control survival.**	Calculated alga acute toxicity values for the eight chemicals representative of substances in the Low 1,3-Butadiene C4 Category are listed below. Commercial substances in this category consist of both high purity hydrocarbons and complex hydrocarbon reaction products with a carbon number distribution that is predominantly C4. The eight chemicals selected to represent the acute toxicity range of this category are C4 hydrocarbons that can be found in substances identified by the eight CAS numbers. Constituents representing category members were selected on the basis of carbon number as identified by the category name, chemistry/structure, measured boiling point ranges for category substances, olefinic process (distillation) knowledge, and percentage of the composition of the represented process streams. The range of toxicity data for substance constituents is an estimate of the potential toxicity of category products. Substance Constituent / Calculated log K_{ow} / Alga Toxicity 96-hr EC50 (mg/L) Isobutane 2.23 18.06 n-Butane 2.31 15.35 Isobutylene 2.23 17.44 cis-Butene-2 2.09 23.19 trans-Butene-2 2.09 23.19 Butene-1 2.17 19.71 1,2-Butadiene 2.06 23.77 1,3-Butadiene 2.03 25.27

	Substance Constituent / Measured* log K_{ow} / Alga Toxicity 96-hr EC50 (mg/L) Isobutane 2.76 6.13 n-Butane 2.89 4.71 Isobutylene 2.34 13.94 cis-Butene-2 2.31 14.81 trans-Butene-2 2.33 14.22 Butene-1 2.40 12.33 1,2-Butadiene na na 1,3-Butadiene 1.99 27.42 na = not available * Experimental K_{ow} values supplied by the KOWWIN program database (EXPKOW.DB) which contains more than 13,000 organic compounds with reliably measured values. The data represent a potential acute toxicity range for substances represented by the 8 CAS numbers under Test Substance.
Test Substance:	The Low 1,3-Butadiene C4 Category includes the following CAS numbers: 106-97-8 Butane 106-98-9 1-Butene 115-11-7 1-Propene,2-methyl 25167-67-3 Butenes 68477-42-9 Gases, petroleum, extractive, C3-5, butene-isobutylene-rich 68477-83-8 Gases, petroleum, C3-5 olefinic-paraffinic alkylation feed 68527-19-5 Hydrocarbons, C1-4, debutanizer fraction 68606-31-5 Hydrocarbons C3-5, butadiene purification by-product Low 1,3-Butadiene C4 Category substances arise from production processes associated with ethylene manufacturing. The eight CAS numbers are used to describe the seven process streams arising from the ethylene process, associated butadiene purification process and other related C4 processes. Four of these process streams are complex mixtures while the remaining three describe high purity

	hydrocarbons. The 1,3-butadiene content is generally less than one percent but on occasion may reach as high as five percent. With the exception of CAS 106-97-8 (butane) these substances contain significant levels of olefins. More information on the Low 1,3-Butadiene C4 Category can be found in the American Chemistry Council, Olefins Panel test plan for this category (1). 1. Olefins Panel, HPV Implementation Task Group. 2001. High Production Volume (HPV) Chemical Challenge Program Test Plan For The Low 1,3-Butadiene C4 Category. American Chemistry Council, Olefins Panel, HPV Implementation Task Group. VA, USA.
Conclusion:	Based on the calculated K_{ow} values, substances in this category are expected to have an alga 96-hour EC50 range of 15.35 to 25.27 mg/L. Based on the measured K_{ow} values, substances in this category are expected to have an alga 96-hour EC50 range of 4.71 to 27.42 mg/L.
Reliability:	(2) Reliable with restrictions The results include calculated data based on chemical structure as modeled by EPIWIN and measured data for specific chemicals as cited in the EPIWIN database. The data represent a potential acute toxicity range for substances with the eight CAS numbers listed under Test Substance. This robust summary has a reliability rating of 2 because the data are not for specific substances in the Low 1,3-Butadiene C4 Category, but rather for selected constituents. These selected constituents represent all substances defined by this category and as such, this robust summary represents a "key study" for a range of acute toxicity to aquatic plants based on constituent data.
Reference:	Cash, G. and V. Nabholz. 1999. ECOSAR Classes for Microsoft Windows, ECOWIN v0.99e. U.S. Environmental Protection Agency, OPPT - Risk Assessment Division. Washington, DC, USA.
Other (source):	American Chemistry Council, Olefins Panel (Prepared 1/03)